

DIGITAL SIMULATION AND OPTIMIZATION OF CATALYTIC REFORMING UNITS

**A Thesis Submitted
In Partial Fulfilment of the Requirements
for the Degree of
MASTER OF TECHNOLOGY**

**By
ASHOK KUMAR SHARMA**

**to the
DEPARTMENT OF CHEMICAL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY KANPUR
MAY 1973**

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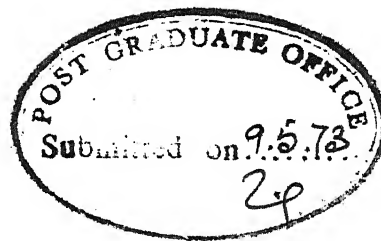
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CERTIFICATE

This is to certify that the present work
'Digital Simulation and Optimization of Catalytic-
Reforming Units' has been carried out under my super-
vision and that this work has not been submitted
elsewhere for a degree.

A handwritten signature in dark ink, appearing to read 'M. Gopala Rao'.

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A. K. Sharma

ABSTRACT

A mathematical model for the simulation of catalytic-reforming units has been developed. The model takes into account most of the complex reactions occurring in the process. The model was used to simulate on a digital computer two industrial Platforming units. Agreement between simulation results and plant data is very satisfactory. It has been found that the performance of an industrial unit can be improved significantly by changing some of the present operating conditions. An optimization routine to minimize the weight of catalyst and the operating cost has been developed. Further work can be done to combine mathematical models of inter heater and a flash unit with the present simulation model.

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ABSTRACT

A mathematical model for the simulation of catalytic-reforming units has been developed. The model takes into account most of the complex reactions occurring in the process. The model was used to simulate on a digital computer two industrial Platforming units. Agreement between simulation results and plant data is very satisfactory. It has been found that the performance of an industrial unit can be improved significantly by changing some of the present operating conditions. An optimization routine to minimize the weight of catalyst and the operating cost has been developed. Further work can be done to combine mathematical models of inter heater and a flash unit with the present simulation model.

CONTENTS

<u>Chapter</u>		<u>Page</u>
	LIST OF FIGURES	vi
	LIST OF TABLES	vii
	NOMENCLATURE	viii
I.	INTRODUCTION	1
II.	LITERATURE ON CATALYTIC REFORMING REACTIONS	7
III.	MATHEMATICAL MODELING AND SIMULATION	11
IV.	OPTIMIZATION	20
V.	RESULTS AND DISCUSSION	34
VI.	CONCLUSIONS AND RECOMMENDATIONS	57
	BIBLIOGRAPHY	59
APPENDIX		
A	PLANT DATA FOR THREE REACTORS SET-UP	60
B	PLANT DATA FOR FOUR REACTORS SET-UP	62
C	HEAT CAPACITIES	64
D	OBJECTIVE FUNCTIONS AND CONSTRAINTS	66
E	COMPUTER PROGRAMME	

LIST OF FIGURES

<u>Figure</u>		<u>Page</u>
1	Catalytic - Reforming Flow Diagram.	5
2	Profiles of, aromatics, hydrogen and hydrocracked products produced, and temperature for Reactor 1.	37
3	Profiles of, aromatics, hydrogen and hydrocracked products produced, and temperature for Reactor 2.	38
4	Profiles of, aromatics, hydrogen and hydrocracked products produced, and temperature for Reactor 3.	39
5	Effect of recycle ratio on yield of aromatics.	41
6	Effect of pressure on yield of aromatics.	42
7	Effect of temperature on conversion of aromatics for $T_1 = 1460^{\circ}\text{R}$.	47
8	Effect of temperature on conversion of hydrogen for $T_1 = 1460^{\circ}\text{R}$.	48
9	Effect of temperature on conversion of hydrocracked products for $T_1 = 1460^{\circ}\text{R}$.	49

LIST OF TABLES

<u>Table</u>		<u>Page</u>
I	SIMULATION RESULTS, COMPARISON OF INDUSTRIAL AND PREDICTED VALUES	35
II	EFFECTS OF TEMPERATURE ON CONVERSION OF AROMATICS, HYDROGEN AND HYDROCRACKED PRODUCT.	43
III	RESULTS FOR MINIMIZATION OF WEIGHT OF CATALYST.	53
IV	RESULTS FOR MINIMIZATION OF OPERATING COST.	54

NOMENCLATURE

A	: Aromatics produced, moles/mole of naphtha
C_p	: Specific heat of the reaction mixture, Btu/(Degree Rankine.mole of feed to the first reactor)
d_p	: Diameter of catalyst particle
d_t	: Diameter of reactor
F_p	: Pounds of feed to first reactor
F_T	: Pound mole of feed to first reactor
G_c	: Force-mass conversion factor
H	: Hydrogen produced, moles/mole of naphtha
HC	: Hydrocracked products produced, moles/mole of naphtha
L	: Length of reactor
M_w	: lb Molecular weight of feed to first reactor
MW_F	: lb Molecular weight of naphtha
N	: Number of reactors in series
N_{Re}	: Reynold's number
P	: Pressure, atm.
P_A	: Partial pressure of aromatics, atm.
P_H	: Partial pressure of hydrogen, atm.
P_N	: Partial pressure of naphthenes, atm.
P_P	: Partial pressure of paraffins, atm.
P_T	: Total pressure, atm.
R	: Gas constant
T	: Temperature, °R

T_i	: Temperature of inlet stream to reactor i.
w	: Weight of catalyst, lb.
w_i	: Weight of catalyst in reactor i, lb.
X_{i5}	: Temperature in reactor i.
X_{ij}	: Extent of conversion for reaction (2.j) in reactor i, mole/mole of feed to first reactor of the series
X_A	: Mole fraction of aromatics in naphtha
X_{AI}	: Mole fraction of aromatics in feed to first reactor
X_{HCI}	: Mole fraction of C_5 and lower hydrocarbons in feed to first reactor
X_{HI}	: Mole fraction of hydrogen in feed to first reactor
X_N	: Mole fraction of naphthenes in naphtha
X_{NI}	: Mole fraction of naphthenes in feed to first reactor
X_P	: Mole fraction of paraffins in naphtha
X_{PI}	: Mole fraction of paraffins in feed to first reactor
ϵ	: Porosity of catalyst bed
e	: Objective function
ρ_c	: Density of catalyst bed, lb/ft ³

CHAPTER I

INTRODUCTION

Use of analogy and simulation has contributed a lot to progress of science and technology. Through analogy with familiar and simple events one can understand more complex phenomena of the world in which one lives. To test analogical conclusions, experiments have to be conducted which simulate the natural conditions one wishes to understand. Because of its very definition, an analogy or simulation can not be identical with realities of nature it attempts to represent.

As technology expands, the demand for laboratory simulation also expands. In some experiments, the parameters which govern the behaviour of the system under study are complex enough to restrain the experimenter from such a work. As a result modern research and technology have found digital and analog simulation not only expedient but also indispensable. And now with the advent of big and fast computers, one can manipulate the mathematical equations of the system, called mathematical model, with a reasonable degree of effort and cost.

Digital simulation is also of vital importance for the chemical industry as it can be used:

1. To facilitate design and operation of process or its parts.
2. To choose operating conditions for changed production pattern or increased production in an existing plant.
3. To study the effect of extreme ranges of operating conditions, some of which might be impractical or impossible to use in a pilot plant.
4. To compress or expand real time.
5. To compare various proposed designs and processes not yet in operation.
6. To test the hypothesis about a system or process before making a decision.
7. To study the effect of changes in variables and parameters with reproducible results.
8. To gain sufficient knowledge about the system to facilitate computer control.

It might appear from the discussion presented above that it is much better to analyse the system by digital-simulation than to analyse it by carrying out laboratory experiments or by pilot-plant studies. Unfortunately, there are certain limitations to the simulation technique as the accuracy of the results obtained by it depends largely on correctness of the mathematical model developed and the accuracy of the physical and chemical data that go into the model.

In India to meet the increasing demand of aromatics (installed capacity of benzene in India has increased from 15,000 tons per annum in 1963 to 87,000 in 1969/70 and the requirements for 1973/74 have been estimated at 1,40,000 tons) a catalytic-reforming plant is being commissioned in Gujrat State. At present the process know-how for this process which uses naphtha as feed stock, is imported from the Western European countries. Catalytic-reforming when combined with solvent extraction or extractive distillation produces, benzene for ultimate conversion to phenol or styrene, toluene for nitration purpose, xylene for plastics etc., in quantities far beyond the capacity of any other source to provide these materials. Catalytic - reforming which goes under various names such as Platforming (Universal Oil Product Co.), Power-forming (Esso Research and Engineering Co.), Ultra-forming (Oil Co. of Indiana), etc. is also used to upgrade the octane number of straight run gasolines, naphtha and other feed stocks. The hydrogen which is liberated in this process can be ploughed back into heavier portion of crude oil either by direct hydrocracking of heavy oil or by milder hydrogenation to produce superior Diesel fuel or improved charge stock to the catalytic cracking units. In order to achieve self-sufficiency (partially or fully) in this important process, it has been intended in the present work to simulate the reactors system coming up in Gujrat State using the IBM 7044 computer.

Catalytic reforming is a high pressure and high temperature process which uses halogenated alumina coated with platinum as catalyst. Generally, three to five steel reactors packed with catalyst with an inter-heater before each are used in series. The reactor vessels are insulated by monolithic ceramic liners. Light gases which have about 85 percent hydrogen are separated in flash unit from catalytic reformat. A part of this gas is used as recycle gas. Detailed process flow diagram is given in Fig. 1.

In the present study, a mathematical model has been developed to predict the product stream of a catalytic-reforming reactor system for a given feed composition, catalyst distribution, inlet temperature, inlet pressure and recycle ratio. The effects of temperature, pressure and recycle ratio have been studied. This mathematical model together with principles of calculus of variation, are used to write an algorithm to extremize an objective function with constraints on final product stream. Using this algorithm, respective objective functions involving total weight of catalyst, and operating costs have been minimized for a three, four, and five reactors set-up.

Present study deals only with the steady state behaviour of the process, dynamic response has not been studied. The composition of recycle gas from the flash unit

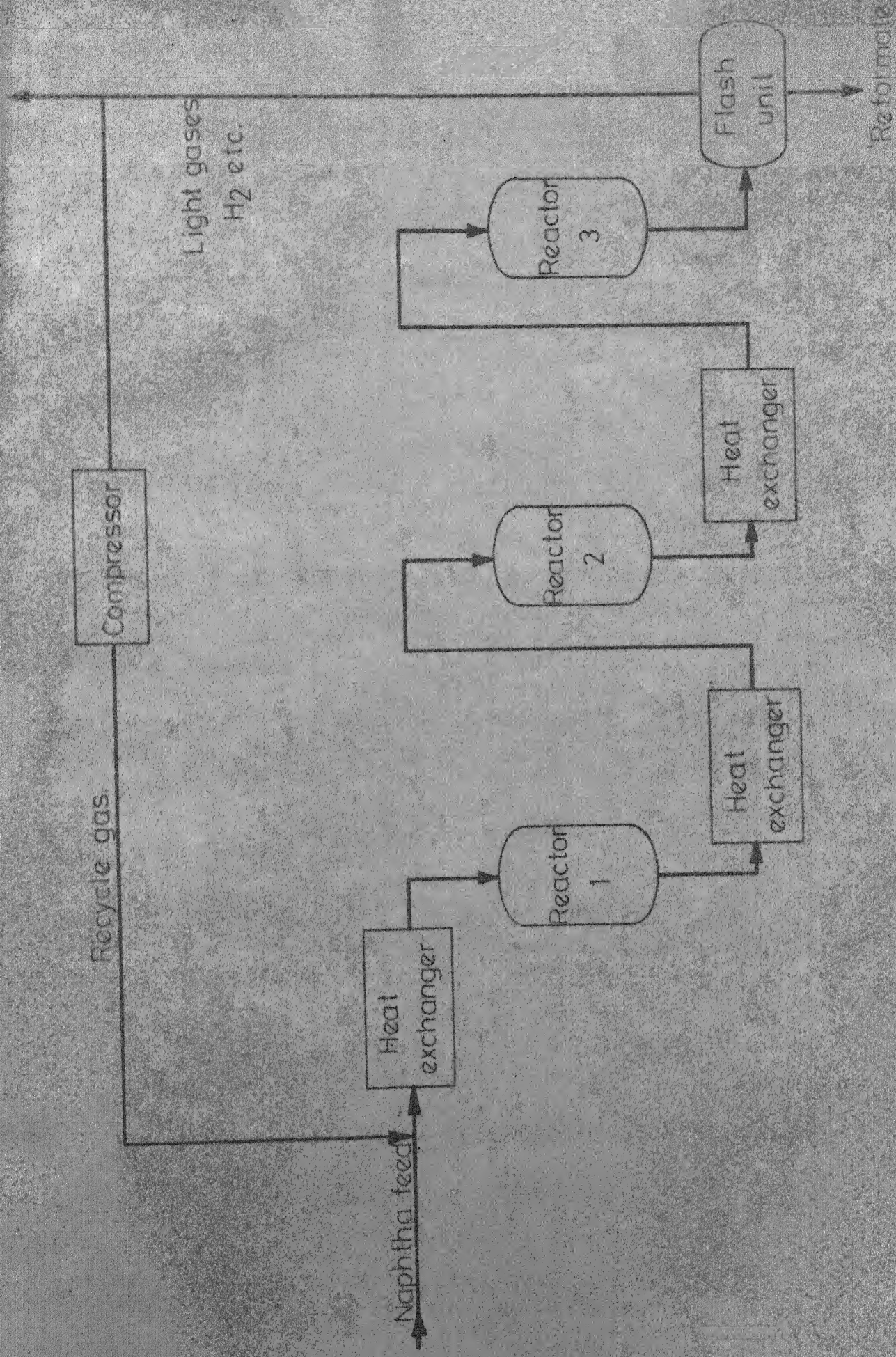


Fig. 1 - Catalytic Reforming Flow Diagram

is not calculated, and instead a fixed composition is assumed. The effect of temperature, pressure and impurities in naphtha on the catalyst life is not considered.

CHAPTER II

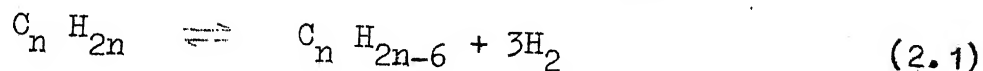
LITERATURE ON CATALYTIC REFORMING REACTION

Many chemical reactions, some simple and some complex, constitute catalytic-reforming but the reactions leading to the formation of aromatics from naphthenes and paraffins are of greater importance. Under the catalytic-reforming conditions, dehydrogenation of naphthenic hydrocarbons is very rapid and contributes substantially for the yield of aromatics. These reactions are highly endothermic and result in somewhat to volumetric shrinkage since the aromatics product is denser than the parent naphthenes (1). Aromatics are also formed from naphthenic intermediate resulting from cyclization of paraffins. But this reaction is not obtained in most ideal sequences because even at a moderate severity level, naphthene dehydrogenation is close to completion while paraffin dehydrocyclization is still in the initial stages. Furthermore for all types of catalyst used commercially, the dehydrocyclization of paraffins is less efficient than dehydrogenation of naphthenes. For this reason, naphthene dehydrogenation to aromatics is considered to be the backbone of catalytic-reforming (2). Hydrocracking which is opposite of dehydrogenation from the stand point of yield and the heat of reaction, is also an important reaction. In this reaction high-molecular weight hydrocarbons decompose to lower-molecular-weight hydrocarbons.

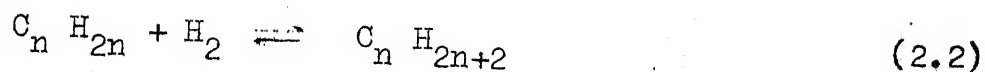
As discussed above, catalytic-reforming is simultaneous dehydrogenation, cyclization and hydrocracking. One can imagine the complexity and cumbersomeness if rate expressions written for each carbon number compounds in the naphtha undergoing the reforming reactions, are to be solved. Kinetic studies have been done by taking each hydrocarbon separately. Attempts have also been made to simplify the problem by treating naphtha to be of some average carbon number depending on its composition. In such studies Smith (3) has come out with a reaction model and rate equations which are reported to be applicable for naphtha feed stocks under widely used operating conditions for catalytic-reforming. Katrush and others (4) report that these kinetic equations fail to predict plant behaviour for Russian naphthas. For each reaction, the rate equations of each reaction used by Katrush et al, for three reactors in series have different rate constants for each reactor. Their results are based on the hypothesis that in the first reactor the main reaction is dehydrogenation, in the second dehydrogenation and cyclization, and in third dehydrocyclization, isomerization and hydrocracking. Recently Heningsen and Nielson (5) have come out with different reaction model and kinetic rate expressions. But these have been reported only for C_8 system and reactions occurring at $500^{\circ}C$ and 30 atm. The rate expression of Marianne Vermorner and others (6) who carried out their work separately

are approximately the same as obtained by Smith. Smith (3) has proposed the following reaction model:

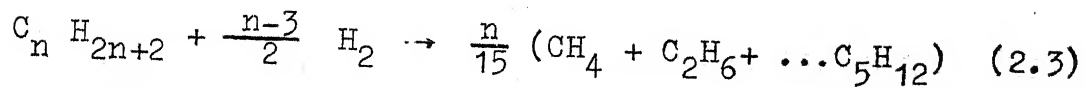
1. Naphthenes \rightleftharpoons Aromatics + Hydrogen



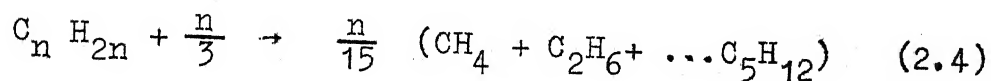
2. Naphthenes + Hydrogen \rightleftharpoons Paraffins



3. Paraffins + Hydrogen \rightarrow Hydrocarbons



4. Naphthenes + Hydrogen \rightarrow Hydrocarbons



In the above reaction model, it has been assumed that the hydrocracking of aromatics is too slow and can be neglected. The stoichiometry of reaction (2.3) and (2.4) which shows that equal number of moles of methane, ethane, propane, butane and pentane are formed from hydrocracking of naphthenes and paraffins, has been derived from experimental observations, that these species are formed approximately in equal molar proportion.

From thermodynamical considerations, one expects catalytic reforming reactions to proceed at low pressures and high temperatures. But at high temperatures, coke gets deposited on the catalyst due to hydrocracking, which reduces the catalyst activity. Coke deposition can be overcome by

having a high hydrogen partial pressure which can be obtained at higher operating pressures. It also reduces sulfur deposition on the catalyst by converting sulfur to hydrogen sulfide (7). Operation at high pressures lengthens the time between regenerations, increases yield of aromatics and reduces the amount of light end products by suppressing hydrocracking. But as the pressure is increased beyond a certain limit, the yield of aromatics deteriorates because of more hydrogenation of naphthenes to paraffins.

Hydrogen partial pressure can also be increased by increasing the hydrogen to hydrocarbon ratio which is direct function of the recycle ratio. Though at low recycle ratio more hydrogen can be formed, the partial pressure of hydrogen is not sufficient to suppress the coke deposition on the catalyst. Increase of hydrogen concentration can also reduce the yield of aromatics because it reverses the order of desirable reactions.

CHAPTER III

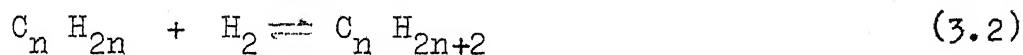
MATHEMATICAL MODELING AND SIMULATION

Assuming that hydrocracking of aromatics to hydrocarbons is negligible and methane, ethane, propane, butane and pentane are formed in equal molar proportions from the hydrocracking of naphthenes and paraffins, one can write the over all reaction model for catalytic - reforming reactions:

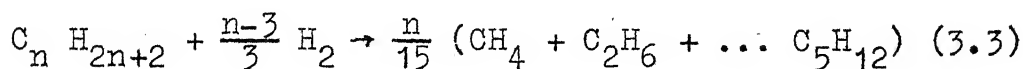
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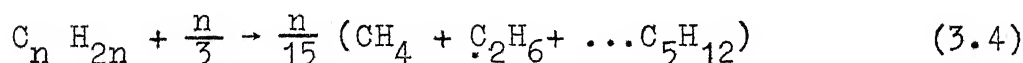
2. Naphthenes + Hydrogen \rightleftharpoons Paraffins



3. Paraffins + Hydrogen \rightarrow Hydrocarbons



4. Naphthenes + Hydrogen \rightarrow Hydrocarbons



Furthermore, it has been found reasonable to assume that each of the three hydrocarbon classes eg. paraffins, naphthenes and aromatics in naphtha, has on the whole the same number of carbon atoms 'n'. Based on this, value of n can be obtained, by expressing molecular weight of naphtha in terms of molecular formula as shown below:

$$XP (C_n H_{2n+2}) + XN (C_n H_{2n}) + XA (C_n H_{2n-6}) = MW_F$$

$$\text{or } n = \frac{1}{14} (MW_F - 2 XP + 6 XA)$$

Experimental data shows that heats of reactions are nearly independent of component molecular weight over the range normally encountered in reforming process, when based on moles of H_2 entering into the reaction. Based on this, kinetic rate expressions and heat of reaction for reactions (2.1) through (2.4) as reported by Smith (3) are given below:

$$1. \quad r_1 = k_1 \left(P_N - \frac{P_A P_H^3}{K_1} \right)$$

$$\frac{\text{lb mole of naphthenes converted to aromatics}}{\text{hr (lb of catalyst)}}$$

(3.5)

$$k_1 = \exp (23.21 - 34750/T) \frac{\text{lb mole naphthenes}}{\text{hr (lb cat) atm}}$$

$$K_1 = \exp (46.15 - 46045/T) \text{ atm}^3$$

$$\Delta H_1 = 30500 \frac{\text{Btu}}{16 \text{ mole } H_2 \text{ produced}}$$

$$2. \quad r_2 = k_2 \left(P_N P_H - \frac{P_P}{K_2} \right)$$

$$\frac{\text{lb mole of naphthenes converted to paraffins}}{(\text{hr. lb cat.})}$$

(3.6)

$$k_2 = \exp (35.98 - 59600/T) \frac{\text{lb mole naphthenes}}{\text{hr. lb cat atm}^2}$$

$$K_2 = \exp (8000/T - 7.12) \text{ atm}^{-1}$$

$$\Delta H_2 = -19000 \frac{\text{Btu}}{16 \text{ mole } H_2 \text{ consumed}}$$

$$3. \quad r_3 = k_3 \frac{P_P}{P_T} \quad (3.7)$$

$$k_3 = \exp(42.97 - 62300/T) \frac{\text{lb mole paraffins}}{\text{hr (lb. cat)}}$$

$$\Delta H_3 = -24300 \frac{\text{Btu}}{\text{mole H}_2 \text{ consumed}}$$

$$4. \quad r_4 = k_4 \frac{P_N}{P_T} \quad (3.8)$$

$$k_4 = \exp(42.97 - 62300/T) \frac{\text{lb mole naphthenes}}{\text{hr. (lb cat)}}$$

$$\Delta H_4 = -22300 \frac{\text{Btu}}{\text{mole H}_2 \text{ consumed}}$$

Under catalytic-reforming conditions for which temperature and pressure are of the order of 800-1000°F and 15-50 atmospheres respectively, the reaction system is always in gaseous state. Preliminary calculations showed that the flow of these gases in the reactors is in highly turbulent region with N_{Re} of the order of 15,000 or more. Since there is sufficient packing on both the sides of reactors, it can be assumed that the flow of gases is in fully developed turbulent flow region in the catalyst zone. Catalytic-reforming reactors also have $L/d_p \gg 20$ and $d_t/d_p > 10$. For such flow conditions and reactors one can safely assume a plug-flow pattern (8).

If X_{i1} , X_{i2} , X_{i3} and X_{i4} are extents of reactions (2.1), (2.2), (2.3) and (2.4); per mole of total feed F_T at a place in reactor i , then the partial pressure terms appearing in the rate equations can be written as follows:

$$\begin{aligned}
P_A &= P_T \text{ mole fraction of aromatics} \\
&= P_T \frac{\text{moles of aromatics}}{\text{Total moles}} \\
&= P_T \frac{X_{AI} + X_{i1}}{1 + 3X_{i1} - X_{i2} + \left(\frac{n}{15} \cdot 5 - 1 - \frac{n-3}{3}\right)X_{i3} + \left(\frac{n}{15} \cdot 5 - 1 - \frac{n}{3}\right)X_{i4}} \\
&= P_T \frac{X_{AI} + X_{i1}}{1 + 3X_{i1} - X_{i2} - X_{i4}} \\
P_N &= P_T \frac{X_{NI} - (X_{i1} + X_{i2} + X_{i4})}{1 + 3X_{i1} - X_{i2} - X_{i4}} \\
P_P &= P_T \frac{X_{PI} + X_{i2} - X_{i3}}{1 + 3X_{i1} - X_{i2} - X_{i4}} \\
P_H &= P_T \frac{X_{HI} + 3X_{i1} - X_{i2} - \frac{n-3}{3}X_{i3} - \frac{n}{3}X_{i4}}{1 + 3X_{i1} - X_{i2} - X_{i4}}
\end{aligned}$$

Material balance for reaction (2.1) for a differential reactor section of catalyst weight Δw , gives:

$$\begin{aligned}
\Delta X_{i1} \cdot F_T &= r_1 \Delta w \\
\text{or } \frac{dX_{i1}}{dw} &= \frac{r_1}{F_T} \\
&= k_1 \left(P_T \frac{(X_{NI} - (X_{i1} + X_{i2} + X_{i4}))}{1 + 3X_{i1} - X_{i2} - X_{i4}} - \right. \\
&\quad \left. \frac{P_T^4 (X_{AI} + X_{i1})(X_{HI} + 3X_{i1} - X_{i2} - \frac{n-3}{3}X_{i3} - \frac{n}{3}X_{i4})^3}{K_1 (1 + 3X_{i1} - X_{i2} - X_{i4})^4} \right) / F_T \quad (3.9)
\end{aligned}$$

For reactions (2.2), (2.3) and (2.4) also similar relations are obtained:

$$\frac{dX_{i2}}{dw} = k_2 \left(\frac{P_T^2 (X_{NI} - X_{i1} - X_{i2} - X_{i4}) (X_{HI} + 3X_{i1} - X_{i2} - \frac{n-3}{3} X_{i3} - \frac{n}{3} X_{i4})}{(1 + 3X_{i1} - X_{i2} - X_{i4})^2} - \frac{P_T (X_{PI} + X_{i2} - X_{i3})}{K_2 (1 + 3X_{i1} - X_{i2} - X_{i4})} \right) / F_T \quad (3.10)$$

$$\frac{dX_{i3}}{dw} = k_3 \frac{(X_{PI} + X_{i2} - X_{i3})}{(1 + 3X_{i1} - X_{i2} - X_{i4}) \cdot F_T} \quad (3.11)$$

$$\frac{dX_{i4}}{dw} = k_4 \frac{(X_{NI} - X_{i1} - X_{i2} - X_{i4})}{(1 + 3X_{i1} - X_{i2} - X_{i4}) F_T} \quad (3.12)$$

Since reactions are carried out in an adiabatic reactor system, energy balance equation can be written as:

$$C_p \cdot F_T \cdot \Delta T = (\Delta X_{i1} \cdot 3(-\Delta H_1) + \Delta X_{i2}(-\Delta H_1) + \Delta X_{i3} \frac{n-3}{3} (-\Delta H_3) + \Delta X_{i4} \frac{n}{3} (-\Delta H_4)) \cdot F_T$$

Dividing both sides of the above equation by Δw , rearranging, and taking the limit $\Delta w \rightarrow 0$, one gets,

$$\frac{dT}{dw} = \left(3 \frac{dX_{i1}}{dw} (-\Delta H_1) + \frac{dX_{i2}}{dw} (-\Delta H_1) + \frac{dX_{i3}}{dw} \frac{n-3}{3} (-\Delta H_3) + \frac{dX_{i4}}{dw} \frac{n}{3} (-\Delta H_4) \right) / C_p \quad (3.13)$$

After manipulating the equation normally used for packed beds (9), pressure drop in the differential element can be written as follows:

$$\frac{dP}{dw} = \frac{(150(1-\epsilon)+1.75)(1-\epsilon) \cdot F_P^2 \cdot R \cdot T \cdot (1+3X_{i1}-X_{i2}-X_{i4})}{\rho_c \cdot \text{Area}^3 \cdot d_p \cdot g_c \cdot \epsilon^3 \cdot M_w \cdot P_T} \quad (3.14)$$

Initial and boundary conditions for reactor system are:

$$X_{1j}(0) = 0 \quad j = 1, 2, 3, 4 \quad (3.15)$$

$$X_{ij}(0) = X_{i-1,j}(W_{i-1}) \quad j = 1, 2, 3, 4 \quad (3.16)$$

$$i = 2, 3, \dots, N$$

Equation (3.9) through (3.14) together with (3.15) and (3.16) constitute the mathematical model for the reactor system.

SIMULATION:

Since fresh feed is mixed with the recycle gas before it is fed to the reactors, the solution of equations (3.9) through (3.14) can not be obtained without knowing the recycle gas composition. Calculations for recycle gas composition are difficult because of two reasons:

Firstly adequate equilibrium data to calculate the composition of the gas separated from product stream of the last reactor in the flash unit are not available.

Secondly some iterative scheme has to be used because of the recycle stream.

The problem can be simplified by assuming recycle gas composition to be the one, normally encountered in catalytic reforming plants. This is justified because of the following reasons:

1. Recycle gas has about 85 percent hydrogen on molar basis.
2. Major portion of the hydrocarbons in the recycle gas is constituted by C_5 and lower hydrocarbons, which do not take part in the reaction model assumed for the present study.

Preliminary calculations also show that a small change in the recycle gas composition does not cause any appreciable effect on the product stream from the reactors.

Specific heat, C_p , occurring in equation (3.13) cannot be treated as constant because the reactions are carried out under adiabatic conditions, and temperature changes are large. Specific heats can be assumed to be linear functions of temperature and it has been found from preliminary calculations that any improvement in this regard does not improve results of simulation to any appreciable extent.

In the specific heat calculations, it was assumed that the carbon-number component break-up of naphthenes, paraffins (higher than C_6) and aromatics in the reaction mixture is the same as it is in the feed to the first reactor. This

assumption was made necessary due to lack of information on the composition (in terms of carbon numbers) of naphthenes, paraffins and aromatics in the product streams. For simplicity, they are lumped together as three species, paraffins, naphthenes and aromatics.

If specific heats of aromatics, naphthenes, paraffins, hydrogen, hydrocarbons coming in feed and hydrocarbons produced by hydrocracking can be represented by the following linear functions of temperature, (details of which appear in Appendix C);

$$C_{pA} = FA(1) + FA(2).T$$

$$C_{pN} = FN(1) + FN(2).T$$

$$C_{pP} = FP(1) + FP(2).T$$

$$C_{pH} = FH(1) + FH(2).T$$

$$C_{pHC} = FHC(1) + FHC(2).T$$

$$C_{pHCl} = FHCl(1) + FHCl(2).T ;$$

the specific heat, C_p , of reaction mixture can be written as,

$$\begin{aligned} C_p = & (XA_I + X_{i1}) C_{pA} + (XN_I - X_{i1} - X_{i2} - X_{i4}) C_{pN} \\ & + (XPI + X_{i2} - X_{i3}) C_{pP} \\ & + (XHI + 3X_{i1} - X_{i2} - \frac{n-3}{3} X_{i3} - \frac{n}{3} X_{i4}) C_{pH} \\ & + (\frac{n}{3} X_{i3} + \frac{n}{3} X_{i4}) C_{pHC} + XHCl. C_{pHCl} \end{aligned}$$

$$\begin{aligned}
\text{or } C_p = & \sum_{j=1}^2 [XAI.FA(j) + XPI.FP(j) + XNI.FN(j) \\
& + XHI.FH(j) + XHCI.FHCI(j) \\
& + (FA(j) - FN(j) + 3.FH(j)) X_{i1} \\
& + (FP(j) - FN(j) - FH(j)) X_{i2} \\
& + (FHC(j) \cdot \frac{n}{3} - FP(j) - FH(j) \cdot \frac{n-3}{3}) X_{i3} \\
& + (FHC(j) \cdot \frac{n}{3} - FN(j) - FH(j) \cdot \frac{n}{3}) X_{i4}] (T)^{j-1}
\end{aligned}$$

Pressure drops along the reactors and inter-heaters in catalytic-reforming plants are of the order of .7 to 1.7 atmospheres. These are small in comparison to the operating pressures. Preliminary calculations show that the results of simulation obtained by assuming the pressure as invariant are approximately the same as those obtained by considering the pressure-drop along length of the reactor. Based on this, equation (3.14) was dropped from the system model i.e. dp/dw has been put equal to zero.

Using the recycle gas composition given in Appendix A, the system equations (3.9) through (3.13) together with (3.15) and (3.16) were solved on the IBM 7044 digital computer by using the fourth-order Runge-Kutta method.

CHAPTER IV

OPTIMIZATION

OBJECTIVE:

Since throughput for a catalytic reforming plant is generally very large, even a small shift in the operating conditions and various parameters of the reactor system from optimum values can change the economic pattern of the process. Reactor sizes, weight of the catalyst, heat exchanger duties and compressor size constitute major share of fixed capital investment, while catalyst life, heat duty and power in-puts to the compressor, determine major part of the operating costs. The variables, temperatures of inlet streams, recycle ratio, operating pressure and number of reactors determine both fixed and operating costs. Higher temperature of the inlet stream though giving rise to higher catalytic activity initially, increases hydrocracking which in turn decreases catalyst activity because of the coke deposition on the catalyst. This can be overcome by having high hydrogen partial pressure which is determined by the choice of the operating pressure and the recycle ratio.

The choice of the operating variables can be subjected to various objectives such as minimization of operating cost or weight of the catalyst for a fixed throughput and fixed

quality of product, or for maximization of venture profit when installing a new plant. Generally constraints on the product are there to ensure certain production rate of aromatics and a certain concentration of these in the reformat. There are also constraints on the lowest and the heighest values of temperature which are determined by reaction rate considerations and catalyst life.

Mathematically, ϵ , the objective function can be function of catalyst weight, catalyst distribution in different reactors, catalyst life, furnace sizes and duties and compressor size and duty.

The constraints are the following:

$$g_1(x_{N1}, x_{N2}, x_{N3}, x_{N4}) = C_1$$

$$g_2(x_{N1}, x_{N2}, x_{N3}, x_{N4}) = C_2$$

$$1260 \leq T_i \leq 1460$$

In the present study, minimization of catalyst weight and minimization of operating cost are the two objective functions seperately investigated. Catalyst life is a variable, which is difficult to take into account. For example the operational life of catalyst depends on temperature, pressure, recycle ratio, and feed composition. Very little data are available in literature. In the present study it is assumed that catalyst is replaced after every 10.8 months. Also, effect of pressure and recycle ratio was not considered in optimization routine.

MATHEMATICAL DEVELOPMENT:

The system under study has reactors in series. Each reactor is represented by five differential equations and is related to the reactor next in the series by four equations. Extremization of an objective function ϵ , for such a system which has constraints also on the final product stream can be done by using Calculus of Variation and Pontryagin principle of optimality (10,11,12,13,14,15).

If W_i is weight of catalyst in reactor i , the reactor system can be described by the following equations:

$$\frac{dX_{ij}}{dW} = f_{ij}$$

or
$$\dot{X}_{ij} = f_{ij} \quad (4.1)$$

X_{ij} corresponds to extent of reaction(2:j)in reactor i for $j = 1,2,3,4$ and

X_{i5} corresponds to temperature in reactor i .

The initial and boundary conditions for (4.1) are,

$$X_{1j}(0) = 0 \quad j = 1,2,\dots,4, \quad (4.2)$$

since reactors are in series

$$X_{i,j}(W_i) = X_{i+1,j}(0) \quad j = 1,2,3,4 \quad (4.3) \\ i = 1,2,\dots, N-1$$

Because of small changes in decision variables the variational equations of the system can be constructed as,

$$\delta \dot{X}_{ij} = \sum_{k=1}^5 \frac{\partial f_{ij}}{\partial X_{ik}} \delta X_{ik} + \text{higher order terms} \quad (4.4)$$

Similarly, variation in the objective function, which may depend on the weight of catalyst and various other parameters of the inlet and outlet stream at each reactor can be written as,

$$\begin{aligned} \delta \varepsilon = & \sum_{l=1}^N \sum_{k=1}^5 \left(\frac{\partial \varepsilon}{\partial X_{lk}(0)} \delta X_{lk}(0) + \frac{\partial \varepsilon}{\partial X_{lk}(W_l)} \delta X_{lk}(W_l) \right) \\ & + \sum_{l=1}^N \frac{\partial \varepsilon}{\partial W_l} \delta W_l + \text{higher order terms} \quad (4.5) \end{aligned}$$

Similarly, variations in the values of constraints, which depend on the outlet stream from the last reactor are,

$$\delta g_1 = \sum_{k=1}^4 \frac{\partial g_1}{\partial X_{Nk}} \delta X_{Nk}(W_N) + \text{higher order terms} \quad (4.6)$$

$$\delta g_2 = \sum_{k=1}^4 \frac{\partial g_2}{\partial X_{Nk}} \delta X_{Nk}(W_N) + \text{higher order terms} \quad (4.7)$$

In the further development, higher order terms have been neglected for the sake of simplicity.

It is readily seen that equations (4.2) and (4.3) for (4.4) become,

$$\delta X_{1j}(0) = 0 \quad j = 1, 2, 3, 4 \quad (4.8)$$

$$\delta X_{i,j}(W_i) = \delta X_{i+1,j}(0) \quad i = 1, 2, \dots, N-1 \quad (4.9)$$

Now multiply Equation (4.4) by arbitrary continuous functions $\lambda_{ij}(w)$ and integrate for $w = 0$ to $w = W_i + \delta W_i$. Thus,

$$\int_0^{W_i + \delta W_i} \lambda_{ij} \dot{\delta X}_{ij} dw = \int_0^{W_i + \delta W_i} \sum_{k=1}^5 \frac{\partial f_{ij}}{\partial X_{ik}} \delta X_{ik} \lambda_{ij} dw \quad (4.10)$$

Integrating left hand side of eqn. (4.10) by parts,

$$\int_0^{W_i + \delta W_i} \lambda_{ij} \dot{\delta X}_{ij} dw = \lambda_{ij} \delta X_{ij} \Big|_0^{W_i + \delta W_i} - \int_0^{W_i + \delta W_i} \dot{\lambda}_{ij} \delta X_{ij} dw \quad (4.11)$$

$$\lambda_{ij} \delta X_{ij} \Big|_0^{W_i + \delta W_i} = \lambda_{ij}(W_i + \delta W_i) \delta X_{ij}(W_i + \delta W_i)$$

$$- \lambda_{ij}(0) \delta X_{ij}(0)$$

$$= \left[\lambda_{ij}(W_i) + \frac{\partial \lambda_{ij}(W_i)}{\partial w} \delta W_i \right]$$

$$\left[\delta X_{ij}(W_i) + \frac{\partial \delta X_{ij}(W_i)}{\partial w} \delta W_i \right]$$

$$- \lambda_{ij}(0) \delta X_{ij}(0)$$

$$= \lambda_{ij}(W_i) \delta X_{ij}(W_i) + \lambda_{ij}(W_i) \cdot$$

$$f_{ij}(W_i) \delta W_i + \dot{\lambda}_{ij}(W_i) \delta W_i \delta X_{ij}(W_i)$$

$$+ \dot{\lambda}_{ij}(W_i) f_{ij}(W_i) \delta W_i \delta W_i$$

$$- \lambda_{ij}(0) \delta X_{ij}(0) \quad (4.12)$$

Neglecting second order terms in (4.12) and making use of (4.11), one gets from equation (4.10)

$$\begin{aligned} & \lambda_{ij}(W_i) \delta X_{ij}(W_i) + \lambda_{ij}(W_i) f_{ij}(W_i) \delta W_i - \lambda_{ij}(0) \delta X_{ij}(0) \\ &= \int_0^{W_i + \delta W_i} \sum_{k=1}^5 \frac{\partial f_{ij}}{\partial X_{ik}} \delta X_{ik} \lambda_{ij} dw + \int_0^{W_i + \delta W_i} \lambda_{ij} \delta X_{ij} dw \end{aligned} \quad (4.13)$$

Now add following to equation (4.5):

1. Equation (4.13) for $i = 1, 2, \dots, N$ and $j = 1, 2, \dots, 5$
2. Multiplications of right hand side of equations (4.6) and (4.7) by arbitrary constants η_1 and η_2 .
3. Multiplications of equation (4.9) with v_{ij} for $i = 1, 2, \dots, N-1$ and $j = 1, 2, 3, 4$.

If \mathcal{E}_1 and \mathcal{E}_2 have fixed values C_1 and C_2 respectively i.e., $\delta \mathcal{E}_1 = \delta \mathcal{E}_2 = 0$.

$$\begin{aligned} \delta \mathcal{E} &= \sum_{l=1}^N \left(\frac{\partial \mathcal{E}}{\partial W_l} + \sum_{k=1}^5 \lambda_{lk}(W_l) f_{lk}(W_l) \right) \delta W_l \\ &+ \sum_{l=1}^{N-1} \sum_{k=1}^4 \left(\lambda_{lk}(W_l) + v_{lk} + \frac{\partial \mathcal{E}}{\partial X_{lk}} \right) \delta X_{lk}(W_l) \end{aligned}$$

$$\begin{aligned}
& + \sum_{k=1}^5 (\lambda_{Nk}(W_N) + \eta_1 \frac{\partial g_1}{\partial X_{Nk}(W_N)} + \eta_2 \frac{\partial g_2}{\partial X_{Nk}(W_N)} \\
& + \frac{\partial \varepsilon}{\partial X_{Nk}(W_N)}) \delta X_{Nk}(W_N) - \sum_{l=1}^{N-1} (\lambda_{l5}(W_l) + \frac{\partial \varepsilon}{\partial X_{l5}(W_l)}) \cdot \\
& \delta X_{l5}(W_l) - \sum_{l=2}^{N-1} \sum_{k=1}^4 (\lambda_{lk}(0) + v_{l-1,k} - \frac{\partial \varepsilon}{\partial X_{lk}}) \cdot \\
& \delta X_{lk}(0) - \sum_{l=1}^N (\lambda_{l5}(0) - \frac{\partial \varepsilon}{\partial X_{l5}(0)}) \delta X_{l5}(0) \\
& - \sum_{k=1}^4 (\lambda_{1k}(0) \delta X_{1k}(0) - \frac{\partial \varepsilon}{\partial X_{1k}(0)}) \delta X_{1k}(0) \\
& - \sum_{l=1}^N \sum_{k=1}^5 \int_0^{W_l + \delta W_l} (\dot{\lambda}_{lk} + \sum_{m=1}^5 \lambda_{lm} \frac{\partial f_{lm}}{\partial X_{lk}}) \delta X_{lk} \cdot dw \quad (4.14)
\end{aligned}$$

There are certain terms which are not at one's disposal, namely, $\delta X_{lk}(W_l)$ in the integrand, $\delta X_{ij}(0)$, $i = 2, \dots, N$, $j = 1, \dots, 4$ and $\delta X_{ij}(W_i)$, $i = 1, 2, 3, 4$, $j = 1, 2, \dots, 5$. Therefore eliminate these terms from the expression for $\delta \varepsilon$, by removing some of the arbitrariness and making them to satisfy the following equations:

$$\begin{aligned}
\dot{\lambda}_{ij} + \sum_{k=1}^5 \lambda_{ik} \frac{\partial f_{ik}}{\partial X_{ij}} &= 0 \quad i = 1, 2, \dots, N \\
& j = 1, 2, \dots, 5 \quad (4.15)
\end{aligned}$$

$$\begin{aligned}
\lambda_{ij}(W_i) + v_{ij} + \frac{\partial \varepsilon}{\partial X_{ij}(W_i)} &= 0 \quad i = 1, 2, \dots, N-1 \\
& j = 1, 2, 3, 4 \quad (4.16)
\end{aligned}$$

$$\lambda_{ij}(0) + v_{i-1,j} - \frac{\partial \varepsilon}{\partial x_{ij}(0)} = 0 \quad i = 1, \dots, N-1$$

$$j = 1, \dots, 4 \quad (4.17)$$

$$\lambda_{i5}(w_i) + \frac{\partial \varepsilon}{\partial w_{i5}(w_i)} = 0 \quad i = 1, 2, \dots, N-1 \quad (4.18)$$

$$\lambda_{Nj}(w_N) + n_1 \frac{\partial g_1}{\partial x_{Nj}(w_N)} + n_2 \frac{\partial g_2}{\partial x_{Nj}(w_N)}$$

$$+ \frac{\partial \varepsilon}{\partial x_{Nj}(w_N)} = 0 \quad j = 1, 2, \dots, 5 \quad (4.19)$$

Combining equations (4.16) and (4.17)

$$\lambda_{ij}(w_i) = \lambda_{i+1,j}(0) - \frac{\partial \varepsilon}{\partial x_{i+1,j}(0)} - \frac{\partial \varepsilon}{\partial x_{ij}(w_i)}$$

$$i = 1, 2, \dots, N-1$$

$$j = 1, 2, 3, 4 \quad (4.20)$$

Equations obtained from (4.15) for the indicated set of i and j are termed as adjoint equations.

Making use of equations (4.8), (4.15) to (4.19), $\delta \varepsilon$ can be written as,

$$\delta \varepsilon = \sum_{l=1}^N \left(\frac{\partial \varepsilon}{\partial w_l} + \sum_{k=1}^5 \lambda_{lk}(w_l) f_{lk}(w_l) \right) \delta w_l$$

$$+ \sum_{l=1}^N \left(\frac{\partial \varepsilon}{\partial x_{l5}(0)} - \lambda_{l5}(0) \right) \delta x_{l5}(0) \quad (4.21)$$

And since δg_1 and δg_2 are assumed to be zero,

$$\sum_{k=1}^5 \frac{\partial g_1}{\partial X_{Nk}} \delta X_{Nk}(W_N) = 0 \quad (4.22)$$

$$\sum_{k=1}^5 \frac{\partial g_2}{\partial X_{Nk}} \delta X_{Nk}(W_N) = 0 \quad (4.23)$$

PROCEDURE:

The optimum for the objective function ϵ can now be approached numerically by using the method of steepest descent. In this method one starts with an arbitrary decision variable vector and approach the optimum by moving in the gradient directions, which are in the direction of minimum. Thus find $\delta \epsilon$ such that

$$\begin{aligned} \epsilon_{\text{new}} &< \epsilon_{\text{old}} \\ \text{or} \quad \delta \epsilon &< 0 \end{aligned} \quad (4.24)$$

This condition (Equation 4.24) which is also necessary condition for minimum, can be met for (4.21), if

$$\delta W_1 = -w^* \left(\frac{\partial \epsilon}{\partial W_1} + \sum_{k=1}^5 \lambda_{1k}(W_1) f_{1k}(W_1) \right) \quad (4.25)$$

$$\delta X_{15}(0) = -w^* \left(\frac{\partial \epsilon}{\partial X_{15}(0)} - \lambda_{15}(0) \right) \quad (4.26)$$

where w^* is a positive weight function.

Then the potential computational scheme will be as follows:

1. For assumed values of various variables which satisfy the system constraints, calculate coefficients of δW_1 and $\delta X_{15}(0)$ for equation (4.21), by solving equations (4.4) and (4.15) together with conditions (4.8), (4.9), (4.18) to (4.20), (4.22) and (4.23).
2. If constraints are violated, decrease the value of w^* such that $w^* > 0$ and all constraints are satisfied.
3. Now define W_1 and $X_{15}(0)$ such that,

$$W_1|_{\text{new}} = W_1|_{\text{old}} - w^* \left(\frac{\partial \epsilon}{\partial W_1} + \sum_{k=1}^5 \lambda_{1k}(W_1) f_{1k}(W_1) \right)$$

$$X_{15}(0)|_{\text{new}} = X_{15}(0)|_{\text{old}} - w^* \left(\frac{\partial \epsilon}{\partial X_{15}(0)} - \lambda_{15}(0) \right)$$

Repeat steps 1, 2 and 3 for new values of W_1 and $X_{15}(0)$ until no further improvement is possible in ϵ .

It may appear that the coefficients of δW_1 and $\delta X_{15}(0)$ in equations (4.21) can be calculated by integrating the equations (4.4) and (4.15), and making use of equations (4.22) and (4.23) together with initial condition and boundary condition (4.18) through (4.20). But, η_1 and η_2 in equation (4.19) cannot be calculated directly by any of the above equations. As in general cases, one can decide to assume certain values for η_1 and η_2 and check whether relations (4.22) and (4.23)

are satisfied after integrating (4.15) and (4.4). In this case one may have to search over the whole range of n_1 and n_2 to satisfy (4.22) and (4.23), because the system of equations do not give any scheme to improve upon the assumed values. The problem is simplified by using Green's function and Green's identity (15) for both Adjoint equations and variational system equations.

Defining Green's function r_{ijk} for Adjoint equations (4.15) by,

$$r_{ijk} = \sum_{l=1}^5 r_{ijl} \frac{\partial f_{il}}{\partial x_{il}} \quad \begin{array}{l} i = 1, 2, \dots, N \\ j \text{ and } k = 1, 2, \dots, 5 \end{array} \quad (4.27)$$

with initial conditions

$$\begin{aligned} r_{ijk}(0) &= \delta_{jk} \\ \text{i.e. } r_{ijk}(0) &= 1 \quad j = k \\ &= 0 \quad j \neq k \end{aligned}$$

The Green's identity for set of equations (4.27) is,

$$\lambda_{ij}(0) = \sum_{k=1}^5 r_{ijk}(w_i) \lambda_{ik}(w_i) \quad (4.28)$$

From (4.19) one has,

$$\begin{bmatrix} \lambda_{N1}(w_N) \\ \lambda_{N2}(w_N) \\ \vdots \\ \lambda_{N5}(w_N) \end{bmatrix} = \begin{bmatrix} \frac{\partial g_1}{\partial x_{N1}} & \frac{\partial g_2}{\partial x_{N1}} & \frac{\partial \epsilon}{\partial x_{N1}} \\ \frac{\partial g_1}{\partial x_{N2}} & \vdots & \frac{\partial \epsilon}{\partial x_{N2}} \\ \vdots & \vdots & \vdots \\ \frac{\partial g_1}{\partial x_{N5}} & \frac{\partial g_2}{\partial x_{N5}} & \frac{\partial \epsilon}{\partial x_{N5}} \end{bmatrix} \begin{bmatrix} -\eta_1 \\ -\eta_2 \\ \vdots \\ -1 \end{bmatrix} \quad (4.29)$$

and from (4.28),

$$\begin{bmatrix} \lambda_{N1}(0) \\ \lambda_{N2}(0) \\ \vdots \\ \lambda_{N5}(0) \end{bmatrix} = \begin{bmatrix} \Gamma_{N11} & \Gamma_{N12} & \cdots & \Gamma_{N15} \\ \Gamma_{N21} & \cdots & \cdots & \Gamma_{N25} \\ \vdots & \vdots & \vdots & \vdots \\ \Gamma_{N51} & \cdots & \cdots & \Gamma_{N55} \end{bmatrix} \begin{bmatrix} \lambda_{N1}(w_N) \\ \lambda_{N2}(w_N) \\ \vdots \\ \lambda_{N5}(w_N) \end{bmatrix} \quad (4.30)$$

Now making use of (4.30) and (4.29), (4.20) gives,

$$\begin{bmatrix} \lambda_{N-1,1}(w_{N-1}) \\ \lambda_{N-1,2}(w_{N-1}) \\ \vdots \\ \lambda_{N-1,5}(w_{N-1}) \end{bmatrix} = \begin{bmatrix} \lambda_{N1}(0) \\ \lambda_{N2}(0) \\ \vdots \\ \lambda_{N5}(0) \end{bmatrix} - \begin{bmatrix} \frac{\partial \epsilon}{\partial x_{N1}(0)} \\ \frac{\partial \epsilon}{\partial x_{N2}(0)} \\ \vdots \\ \frac{\partial \epsilon}{\partial x_{N5}(0)} \end{bmatrix} - \begin{bmatrix} \frac{\partial \epsilon}{\partial x_{N-1,1}(w_{N-1})} \\ \frac{\partial \epsilon}{\partial x_{N-1,2}(w_{N-1})} \\ \vdots \\ \frac{\partial \epsilon}{\partial x_{N-1,5}(w_{N-1})} \end{bmatrix} \quad (4.31)$$

$$= \begin{bmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & \vdots & A_{23} \\ \vdots & \vdots & \vdots \\ A_{51} & A_{52} & A_{53} \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ 1 \end{bmatrix}$$

and it is readily seen that A_{ij} can be expressed in terms of coefficients of, first matrix of right hand side of (4.29), first matrix of right hand side of (4.30) and second and third matrices of right hand side of (4.31).

With the above procedure other values of $\lambda_{ij}(0)$ and $\lambda_{ij}(W_i)$ can be known in terms of n_1 and n_2 and thus coefficients of $\delta X_{15}(0)$ and δW_1 in (4.19) can be known in terms of n_1 and n_2 .

Now to calculate values of $\delta X_{Nj}(W_N)$ in terms of n_1 and n_2 which will be used to evaluate n_1 and n_2 from equations (4.22) and (4.23), one writes Green's functions for the Variational System Equation;

$$\begin{aligned} r_{ijk} = - \sum_{l=1}^5 r_{ijl} \frac{\partial f_{il}}{\partial X_{ij}} \quad i = 1, 2, \dots, N \quad (4.32) \\ j \text{ and } k = 1, 2, \dots, 5 \end{aligned}$$

with boundary conditions

$$\begin{aligned} r_{ijk}(W_i) &= 1 & j &= k \\ &= 0 & j &\neq k \end{aligned}$$

Greens identity for (4.32) is,

$$\delta X_{ij}(W_i) = \sum_{k=1}^5 r_{ijk}(0) \delta X_{ik}(0) \quad (4.33)$$

And since there is also a δW_1 change in weight of catalyst W_1 ,

$$\begin{bmatrix} \delta X_{11}(W_1) \\ \delta X_{12}(W_1) \\ \cdot \\ \cdot \\ \delta X_{14}(W_1) \end{bmatrix} = \begin{bmatrix} \Gamma_{111} & \Gamma_{112} & \dots & \Gamma_{115} \\ \Gamma_{121} & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \Gamma_{141} & \Gamma_{142} & & \Gamma_{145} \end{bmatrix} \begin{bmatrix} \delta X_{11}(0) \\ \delta X_{12}(0) \\ \cdot \\ \cdot \\ \delta X_{15}(0) \end{bmatrix} + \begin{bmatrix} f_{11} \cdot \delta W_1 \\ f_{12} \cdot \delta W_1 \\ \cdot \\ \cdot \\ f_{14} \cdot \delta W_1 \end{bmatrix}$$

$$= \begin{bmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ B_{41} & B_{42} & B_{43} \end{bmatrix} \begin{bmatrix} \eta_1 \\ \eta_2 \\ 1 \end{bmatrix}$$

Here again coefficients B_{ij} can be easily calculated.

Making use of (4.9) and following the above procedure $\delta X_{Nj}(W_N)$ can be calculated in terms of η_1 and η_2 . And now substituting the values of $\delta X_{Nj}(W_N)$ in (4.22) and (4.23), η_1 and η_2 can be calculated.

CHAPTER V

RESULTS AND DISCUSSION

In Table I, the outputs from the model are compared with those from the two industrial plants. The details of each plant e.g., weight of catalyst in each reactor, feed and recycle gas composition, feed rate, recycle ratio, and temperatures and pressure of inlet streams are given in Appendices A and B. Though not all the desired data is available for the industrial reactors, comparison was made with two types of industrial units. One unit has three reactors in series and the other has four reactors in series. The amount of aromatics and paraffins in stream leaving the reactor were predicted with in 7.7 percent and 4.7 percent respectively for the two cases. The temperature of exit streams were also predicted by the model within 1.8 percent. Production rate of hydrogen and hydrocracked products were predicted with in 2.1 percent. The prediction of naphthenes conversion was not satisfactory. A vain attempt was made to increase the accuracy of the results, by changing the rate constants appearing in equations (3.5) through (3.8). However, as the significant characteristics of the reactor systems have been predicted satisfactorily, it can be assumed that the proposed model represents very well the true behaviour of the plants.

TABLE I: SIMULATION RESULT, COMPARISON OF INDUSTRIAL AND PREDICTED VALUES.

 I_A and I_B = Industrial

P = Predicted

E = Error %

Reactor Set-up	Stream leaving reactor	Aroma- ties lb m/hr	Naph- thenes lb m/hr	Para- ffins lb m/hr	H ₂ pro- duced lb m/hr	Hydro- cracked product lb m/hr	Temperature °R
Three in Series	I_A						1255.
	1 P						1288.9
	E						1.3
	I_A						1320.
	2 P						1330.
	E						.8
	I_A	170.	8.9	76.5			1400.
	3 P	157.	2.5	77.4			1374.5
	E	7.7	73.0	1.2			1.8
Four in Series	I_B	74.7	80.0	76.0			1271.
	1 P	73.9	79.31	77.			1281.
	E	1.1	.9	1.3			.8
	I_B	109.	39.6	79.2			1318.
	2 P	108.	38.	82.			1322.
	E	.7	4.0	3.5			.3
	I_B	129.4	12.7	75.0			1368.
	3 P	126.	11.55	78.5			1380.
	E	2.6	10.0	4.7			.9
	I_B	140.1	4.9	42.5	252.	122.5	1409.
	4 P	137.6	5.07	45.6	244.6	119.9	1406.
	E	1.7	21.8	.73	2.1	2.1	.2

The profiles of conversions to aromatics, hydrogen and hydrocracked products and temperature for the plant of Appendix A are shown in Figures 2,3 and 4. It can be seen that in reactor 1 and 2, dehydrogenation of naphthenes to aromatics is dominant (Figures 2 and 3) and since this reaction is endothermic, temperature along the reactor length goes down. It can also be seen from Figure 3 that in reactor -2 more of hydrocracked product is formed than in reactor -1 because of high operating temperature in the reactor-2. Production of aromatics in the reactor -2 is less than in the reactor -1, because dehydrogenation of naphthenes to aromatics is reaching equilibrium, even though the temperature of inlet stream and average operating temperature are higher for reactor -2.

From Figure 4, it can be seen that the conversion of hydrocracked product is dominant and that production of aromatics is very slow in reactor -3. One might expect the temperature to go up and concentration of hydrogen to go down. But the results are contrary. The reaction (2.2), which is endothermic and consumes hydrogen in the forward direction, actually takes place in the backward direction in this reactor. For example extent of reaction (2.2) at the entrance of reactor -3 is .000526 and at the exit it is -.008788.

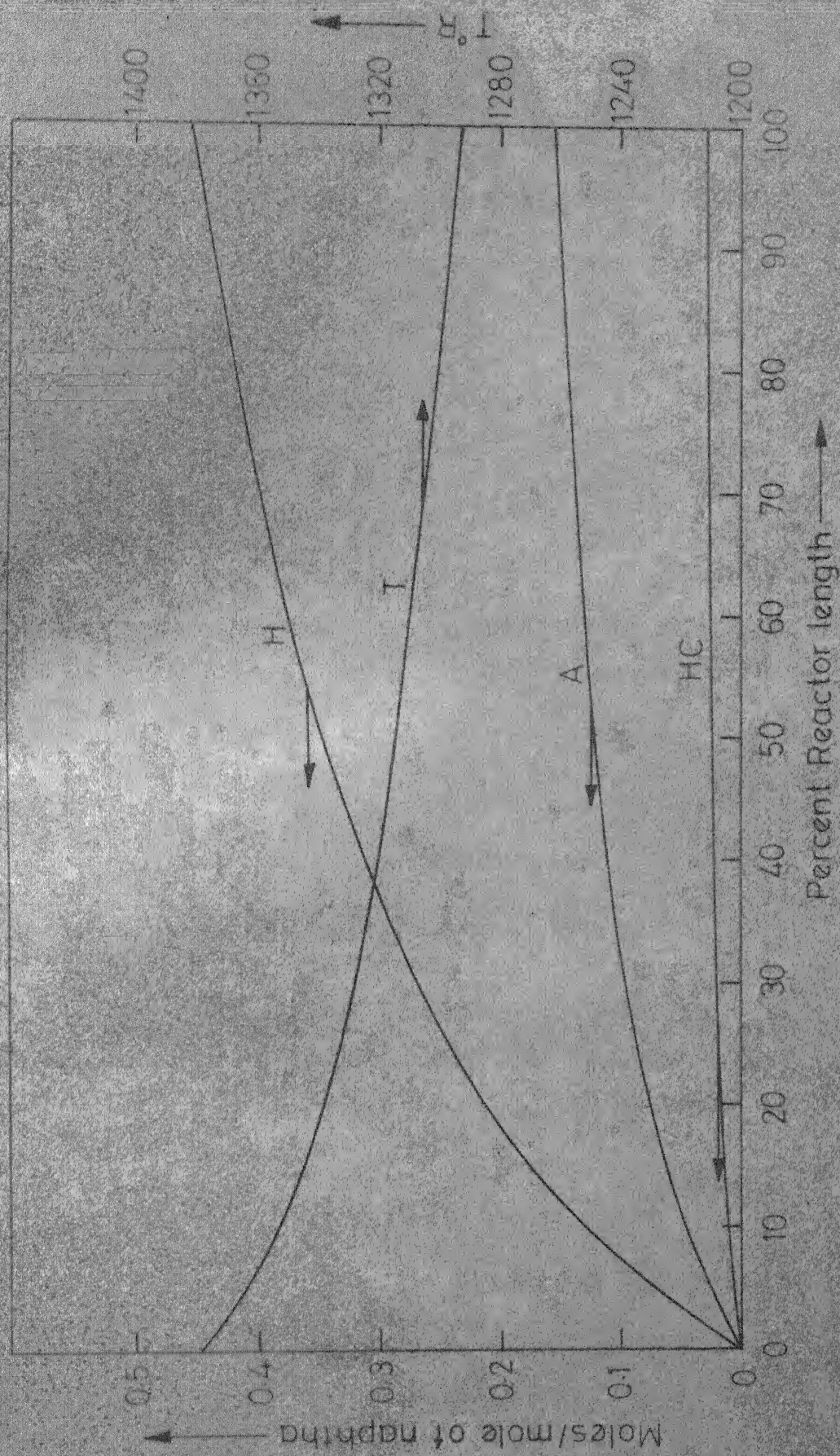


Fig 2 - Profiles of aromatics, hydrogen and hydrocracked products produced, and temperature for Reactor 1

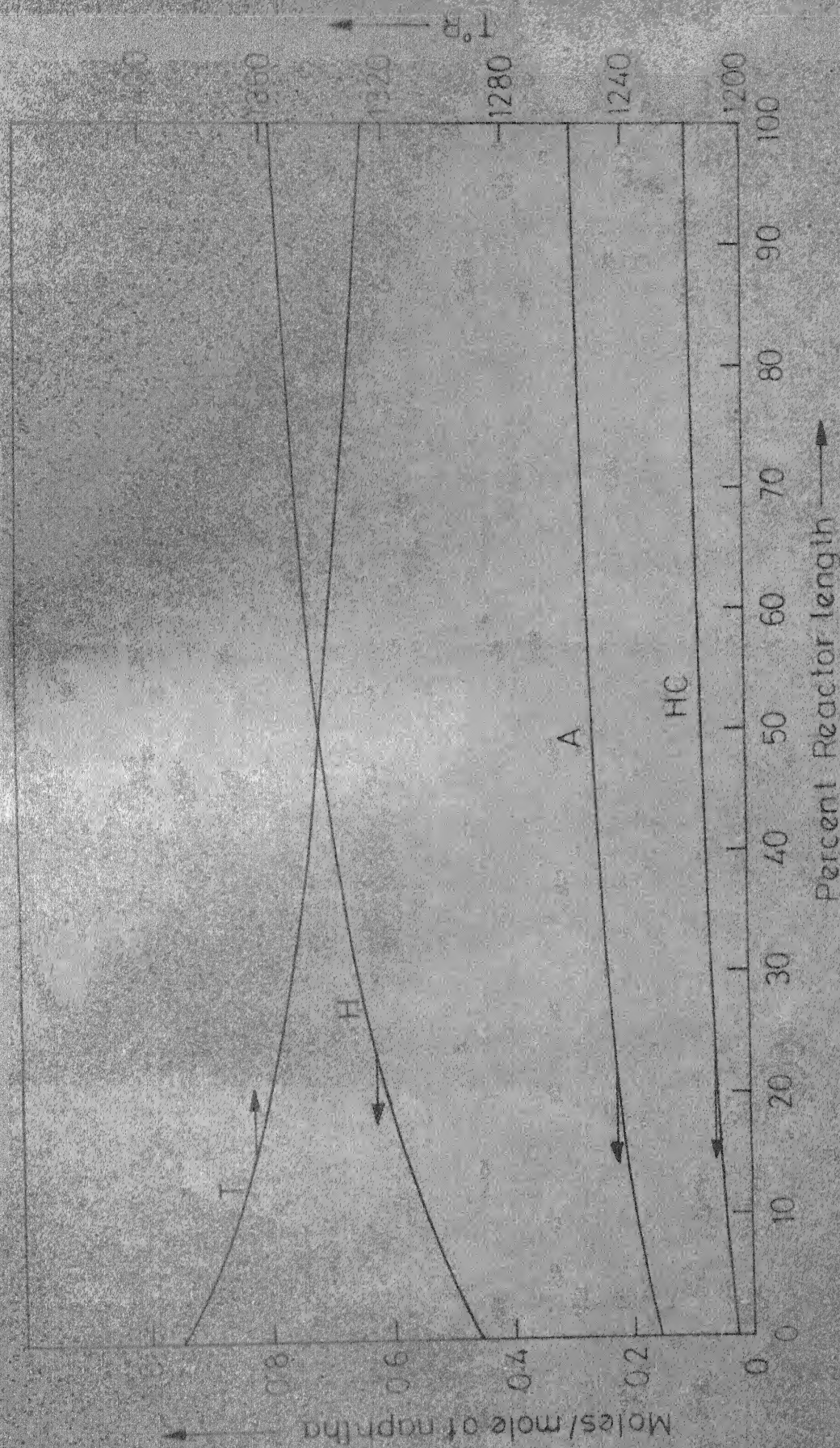


Fig. 3 - Profiles of aromatics, hydrogen and hydrocracked products produced and temperature for Reactor 2

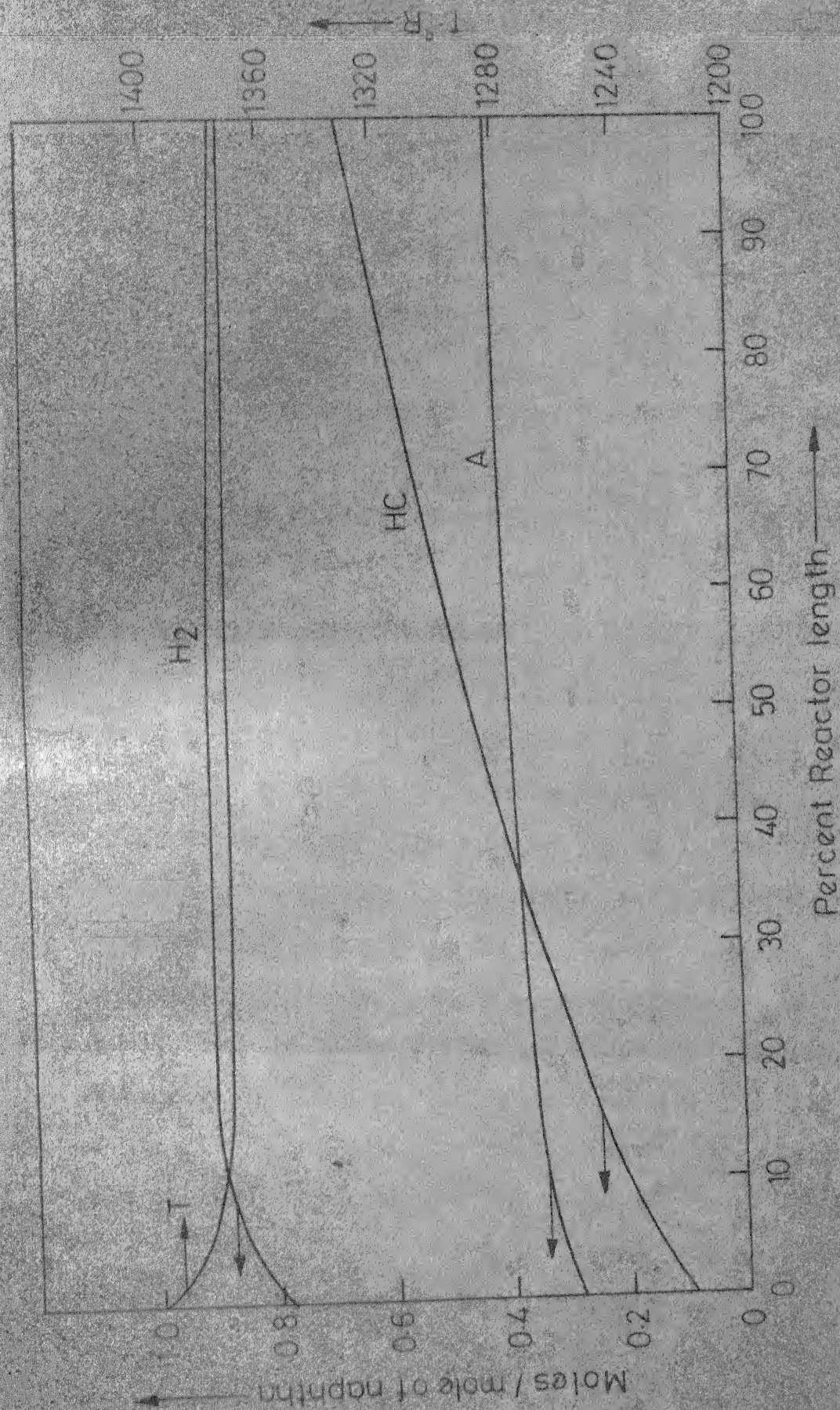


Fig. 4 - Profiles of aromatic, hydrogen and hydrocracked products produced, and temperature for Reactor 3.

SIMULATION RESULTS:

The simulation model was used to study the effect of recycle ratio, and pressure on the production of aromatics. The results are presented in Figures 5 and 6. The effect of the inlet temperatures of the streams on the production of aromatics, hydrogen and hydrocracked product were also studied. The results are given in Table II and Figures 7, 8 and 9. Additional plant data is taken from Appendix A.

(i) Effect of Recycle Ratio:

It can be seen from Figure 5 that as the recycle ratio rises, from 3 to 8, the production of aromatics also rises from .3336 to .4018 mole of aromatics per mole of naphtha, and as it increases from 8 to 10 the production of aromatics remains almost steady. Since reaction (2.1) produces hydrogen in the forward direction, one can expect that the aromatic production rate will go down with the rise in recycle ratio, as the increase in its value increases the partial pressure of hydrogen. But the results are contrary. As the hydrogen partial pressure in the reaction mixture rises because of rise in the recycle ratio, the exothermic reaction (2.2) becomes fast. The temperature rise because of more heat produced in reaction (2.2) is sufficient enough to off set the decrease in the reaction rate of reaction (2.1). It can be further noted from Figure 5 that as recycle ratio rises,

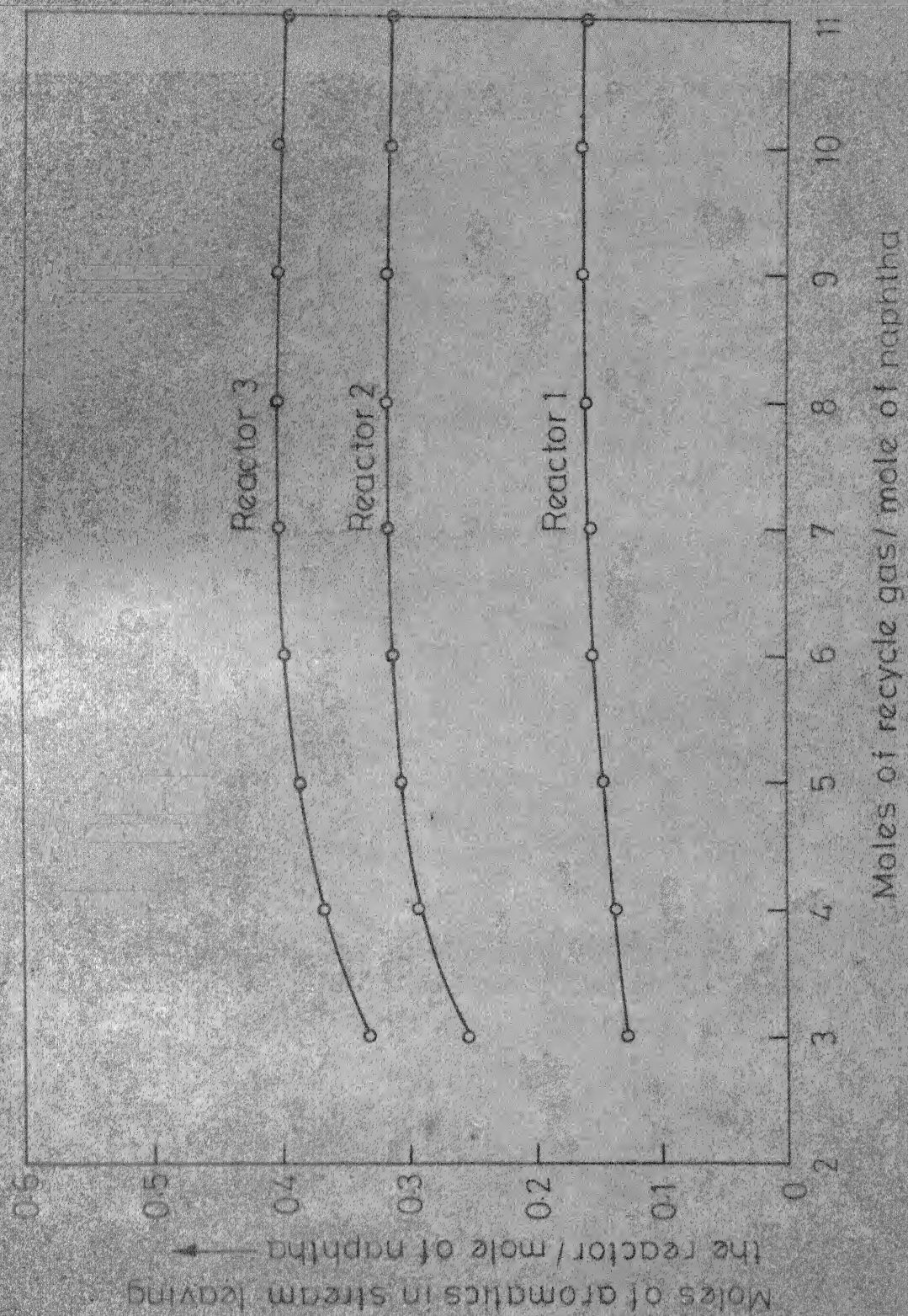


Fig 5 - Effect of recycle ratio on yield of aromatics.

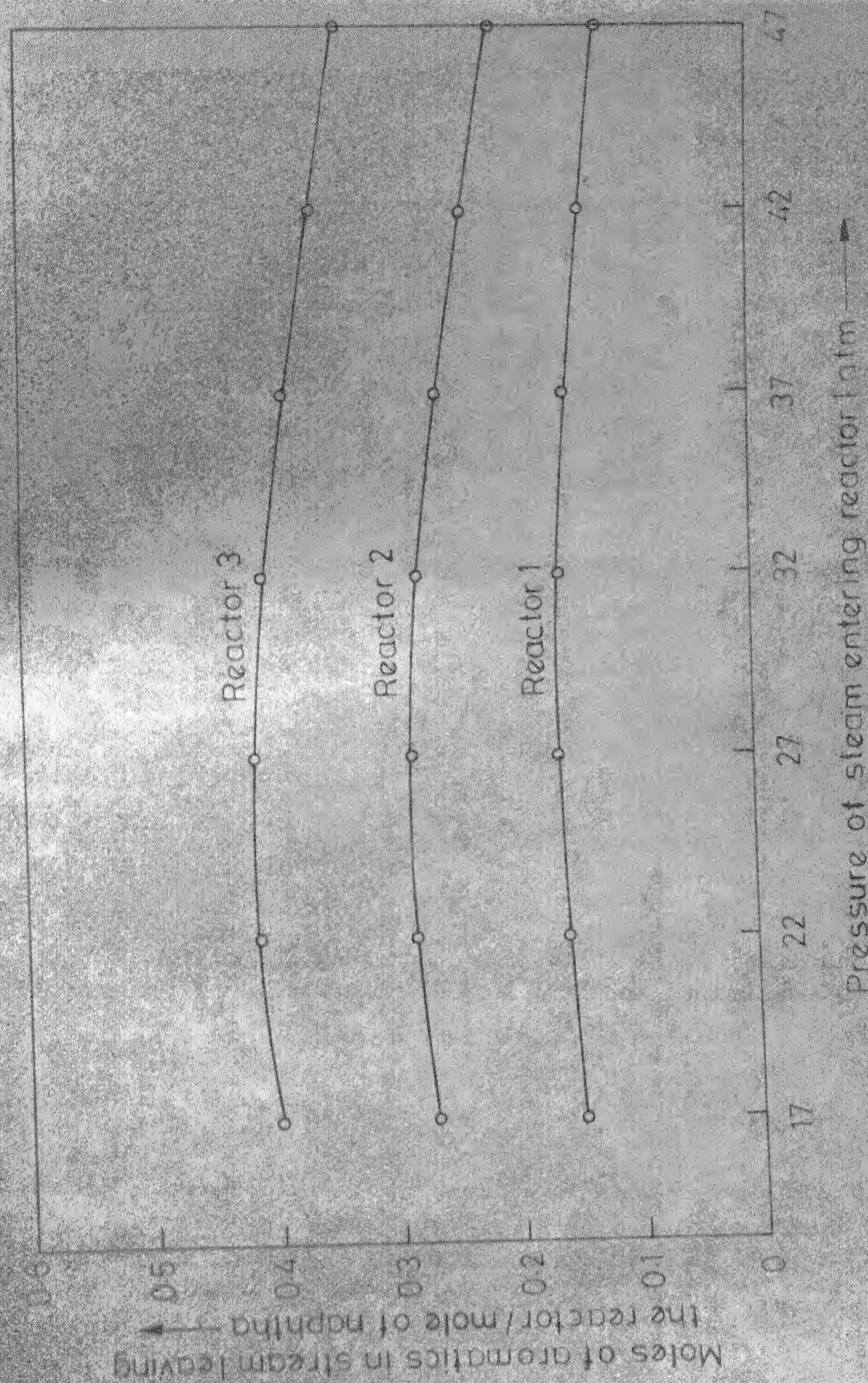


Fig 6 - Effect of pressure on yield of aromatics

TABLE II: EFFECT OF TEMPERATURE ON CONVERSION OF AROMATICS, HYDROGEN AND HYDROCRACKED PRODUCTS.

T ₁	Conversion in Reactor 1	T ₂	Conversion in Reactor 2	Conversion in Reactor 3 for					
				T ₃ = 1285.	T ₃ = 1320.	T ₃ = 1355.	T ₃ = 1390.	T ₃ = 1425.	T ₃ = 1460.
1285.	.0559 .1644 .0032	1285.	.1093	.1978	.2381	.2759	.3093	.3384	.3834
			.3209	.5764	.6882	.7846	.8516	.8660	.8014
			.0072	.0192	.0315	.0561	.1087	.2366	.6074
		1320.	.1437	.2201	.2585	.2937	.3243	.3553	.4123
			.4191	.6372	.7423	.8282	.8791	.8762	.8167
			.0129	.0268	.0413	.0718	.1406	.3169	.7647
		1355.	.1824	.2437	.2795	.3113	.3399	.3785	.4461
			.5251	.6868	.7921	.8630	.8938	.8772	.8309
			.0248	.0414	.0599	.1009	.2005	.4575	.9539
		1390.	.2228	.2663	.2986	.3270	.3575	.4101	.4748
			.6280	.7442	.8259	.8775	.8884	.8689	.8382
			.0484	.0691	.0942	.1549	.3107	.6682	1.1223
		1425.	.2626	.2857	.3141	.3409	.3801	.4438	.4888
			.7135	.7660	.8305	.8615	.8604	.8494	.8280
			.0948	.1216	.1585	.2541	.4839	.9107	1.2247
	.0910 .2649 .0079	1460.	.2991	.3014	.3264	.3555	.4052	.4654	.4867
			.7597	.7462	.7931	.8090	.8077	.8072	.7883
			.1907	.2250	.2786	.4220	.7342	1.1121	1.2731
		1285.	.1375	.2160	.2548	.2904	.3215	.3520	.4069
			.4009	.6257	.7321	.8199	.8738	.8736	.8126
			.0120	.0255	.0396	.0689	.1344	.3010	.7370
		1320.	.1701	.2364	.2731	.3060	.3351	.3705	.4357
			.4936	.6807	.7795	.8556	.8930	.8799	.8287
			.0181	.0337	.0508	.08780	.1756	.4038	.8925
		1355.	.2069	.2580	.2918	.3216	.3506	.3911	.4653
			.5935	.7335	.8214	.8815	.9002	.8804	.8435
			.0310	.0499	.0719	.1230	.2518	.5684	1.0546
		1390.	.2451	.2783	.3086	.3359	.3702	.4298	.4865
			.6888	.7729	.8463	.8874	.8909	.8747	.8474
			.0572	.0809	.1114	.1877	.3843	.7832	1.1762
1320.	.0910 .2649 .0079	1425.	.2822	.2958	.3226	.3502	.3948	.4593	.4936
			.7639	.7860	.8427	.8662	.8637	.8577	.8379
			.1103	.1406	.1848	.3016	.5802	.9946	1.2386
		1460.	.3161	.3113	.3356	.3560	.4179	.4738	.4890
			.7955	.7596	.8017	.8149	.8153	.8173	.7988
			.2234	.2601	.3198	.4782	.8018	1.1487	1.2709

contd..44

T ₁	Conversion in Reactor 1	T ₂	Conversion in Reactor 2	Conversion in Reactor 3 for					
				T ₃ = 1285.	T ₃ = 1320.	T ₃ = 1355.	T ₃ = 1390.	T ₃ = 1425.	T ₃ = 1460.
1355.	.1310 .3763 .0175	1285.	.1692	.2355	.2721	.3050	.3340	.3695	.4348
			.4873	.6743	.7729	.8487	.8858	.8724	.8214
			.0217	.0374	.0544	.0916	.1798	.4091	.8983
		1320.	.1994	.2535	.2878	.3182	.3469	.3911	.4598
			.5724	.7216	.8117	.8748	.8968	.8774	.8479
			.0284	.0466	.0675	.1155	.2354	.5356	1.0290
		1355.	.2334	.2723	.3038	.3317	.3637	.4198	.4818
			.6638	.7656	.8438	.8908	.8981	.8798	.8519
			.0429	.0649	.0925	.1597	.3333	.7124	1.1440
		1390.	.2686	.2900	.3183	.3454	.3857	.4503	.4943
			.7485	.7953	.8588	.8888	.8874	.8772	.8561
			.0732	.1008	.1391	.2386	.4865	.9077	1.2143
		1425.	.3024	.3058	.3313	.3606	.4105	.4726	.4961
			.8096	.7991	.8477	.8648	.8632	.8621	.8430
			.1369	.1713	.2246	.3666	.6779	1.0706	1.2461
		1460.	.3343	.3231	.3468	.3779	.4298	.4802	.4907
			.8238	.7686	.8072	.8189	.8212	.8246	.8068
			.2782	.3162	.3796	.5461	.8670	1.1766	1.2685
1390.	.1738 .4883 .0361	1285.	.2022	.2541	.2880	.3178	.3467	.3927	.4611
			.5700	.7126	.8006	.8610	.8800	.8600	.8228
			.0405	.0592	.0810	.1316	.2591	.5734	1.0607
		1320.	.2291	.2691	.3007	.3286	.3604	.4159	.4785
			.6455	.7507	.8295	.8772	.8851	.8664	.8380
			.0479	.0697	.0968	.1627	.3300	.7087	1.1454
		1355.	.2596	.2849	.3137	.3408	.3792	.4429	.4914
			.7253	.7843	.8509	.8842	.8838	.8715	.8496
			.0647	.0911	.1269	.2189	.4512	.8704	1.2068
		1390.	.2909	.3000	.3263	.3547	.4023	.4669	.4968
			.7960	.8035	.8566	.8770	.8746	.8709	.8515
			.1015	.1340	.1826	.3118	.6103	1.0214	1.2372
		1425.	.3210	.3152	.3397	.3709	.4242	.4809	.4961
			.8394	.7996	.8414	.8544	.8550	.8574	.8387
			.1826	.2208	.2827	.4467	.7787	1.1299	1.2521
		1460.	.3534	.3379	.3608	.3908	.4396	.4839	.4913
			.8377	.7703	.8075	.8192	.8228	.8265	.8096
			.3685	.4051	.4667	.6271	.9265	1.1968	1.2677

Contd...45

T ₁	Conversion in Reactor 1	T ₂	Conversion in Reactor 2	Conversion in Reactor 3 for					
				T ₃ = 1285.	T ₃ = 1320.	T ₃ = 1355.	T ₃ = 1390.	T ₃ = 1425.	T ₃ = 1460.
1425.	.2170 .5890 .0717	1285.	.2344	.2701	.3006	.3278	.3612	.4198	.4779
			.6380	.7296	.8041	.8464	.8505	.8335	.8079
			.0763	.0993	.1288	.2021	.3916	.7848	1.1883
		1320.	.2572	.2817	.3102	.3371	.3760	.4400	.4868
			.7006	.7572	.8225	.8543	.8533	.8417	.8201
			.0847	.1113	.1478	.2419	.4793	.8900	1.2247
		1355.	.2829	.2942	.3206	.3488	.3954	.4605	.4925
			.7653	.7797	.8340	.8553	.8527	.8481	.8287
			.1049	.1367	.1837	.3087	.6014	1.0171	1.2459
		1390.	.3095	.3072	.3321	.3629	.4160	.4758	.4942
			.8180	.7894	.8332	.8471	.8467	.8481	.8292
			.1520	.1894	.2492	.4082	.7404	1.1127	1.2554
		1425.	.3370	.3243	.3481	.3799	.4320	.4831	.4930
			.8424	.7821	.8197	.8309	.8337	.8376	.8198
			.2618	.3012	.3672	.5400	.8674	1.1746	1.2625
		1460.	.3751	.3571	.3788	.4056	.4479	.4850	.4902
			.8335	.7611	.7988	.8117	.8157	.8186	.8032
			.5096	.5413	.5945	.7328	.9898	1.2161	1.2711
1460.	.2584 .6611 .1415	1285.	.2640	.2819	.3089	.3358	.3181	.4423	.4799
			.6748	.7108	.7695	.7947	.7921	.7844	.7643
			.1464	.1749	.2160	.3244	.5887	1.0037	1.2686
		1320.	.2814	.2901	.3158	.3441	.3919	.4554	.4833
			.7214	.7278	.7790	.7978	.7953	.7923	.7731
			.1559	.1883	.2375	.3689	.6698	1.0733	1.2759
		1355.	.3013	.2996	.3242	.3548	.4077	.4672	.4854
			.7669	.7402	.7835	.7969	.7964	.7979	.7792
			.1810	.2179	.2774	.4361	.7673	1.1379	1.2791
		1390.	.3229	.3121	.3359	.3682	.4225	.4750	.4860
			.7990	.7438	.7813	.7921	.7944	.7984	.7803
			.2440	.2839	.3510	.5272	.8639	1.1854	1.2809
		1425.	.3510	.3348	.3574	.3873	.4359	.4791	.4859
			.8092	.7397	.7760	.7873	.7911	.7951	.7786
			.3959	.4323	.4943	.6554	.9527	1.2157	1.2825
		1460.	.3991	.3791	.3992	.4214	.4544	.4825	.4856
			.8061	.7315	.7704	.7849	.7891	.7905	.7770
			.7039	.7283	.7690	.8746	1.0723	1.2443	1.2837

Contd...46

How to read the table:

Upper, middle and lower numerical values of the three figures appearing together in the columns of 'conversion in reactor' stand for aromatics, hydrogen and hydrocracked product, produced per mole of naphtha respectively. For example, aromatics, hydrogen and hydrocracked product produced per mole of naphtha in the stream leaving, reactor one for $T_1 = 1285$ are .0559, .1644 and .0032, reactor two for $T_1 = 1285$, $T_2 = 1320$ are .1437, .4191 and .0129, and reactor three for $T_1 = 1285$, $T_2 = 1320$ and $T_3 = 1355$ are .2937, .8282 and .0718.

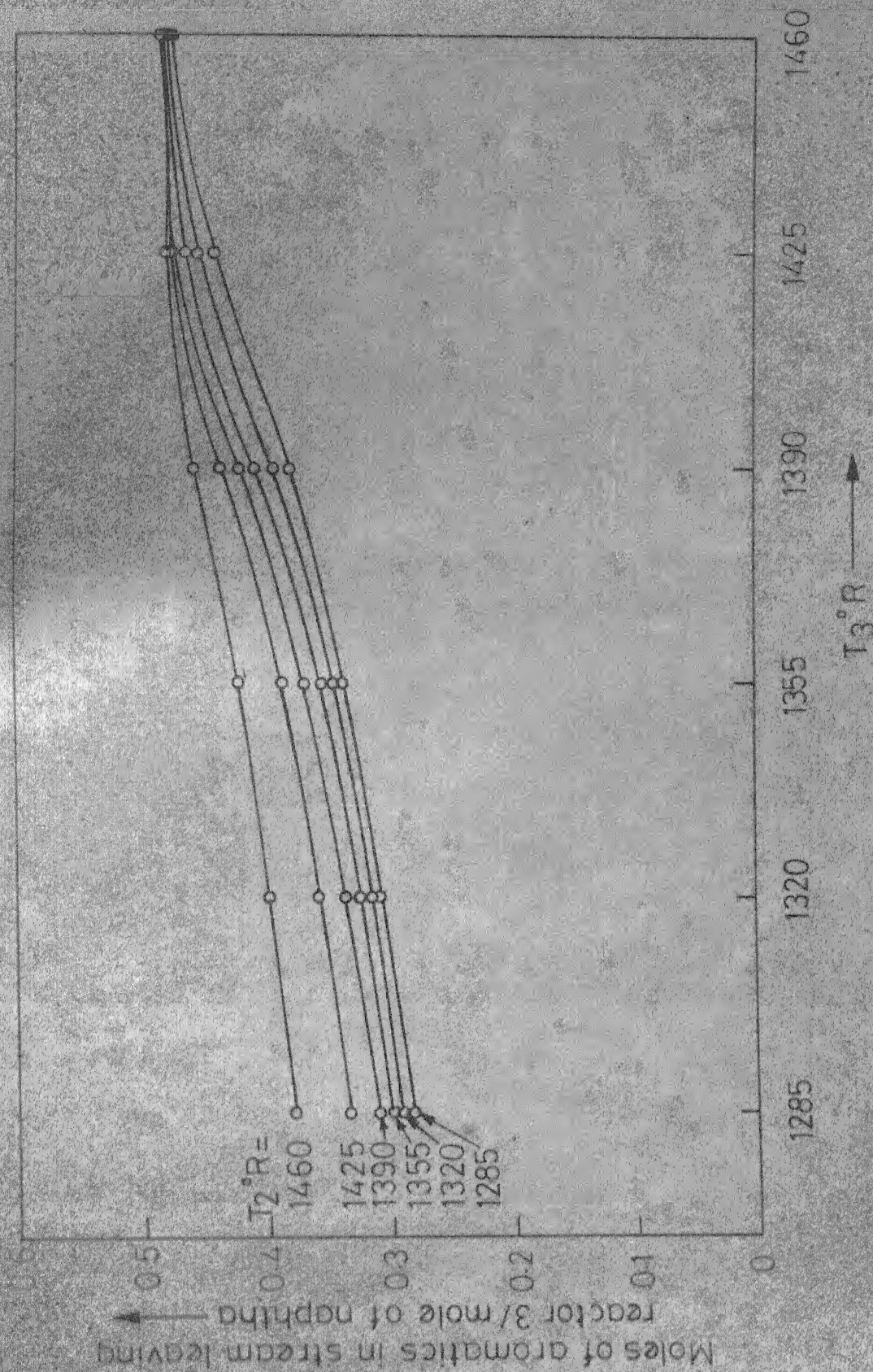


Fig. 7 - Effect of temperature on conversion of aromatics for $T_1 = 1460^{\circ}\text{R}$

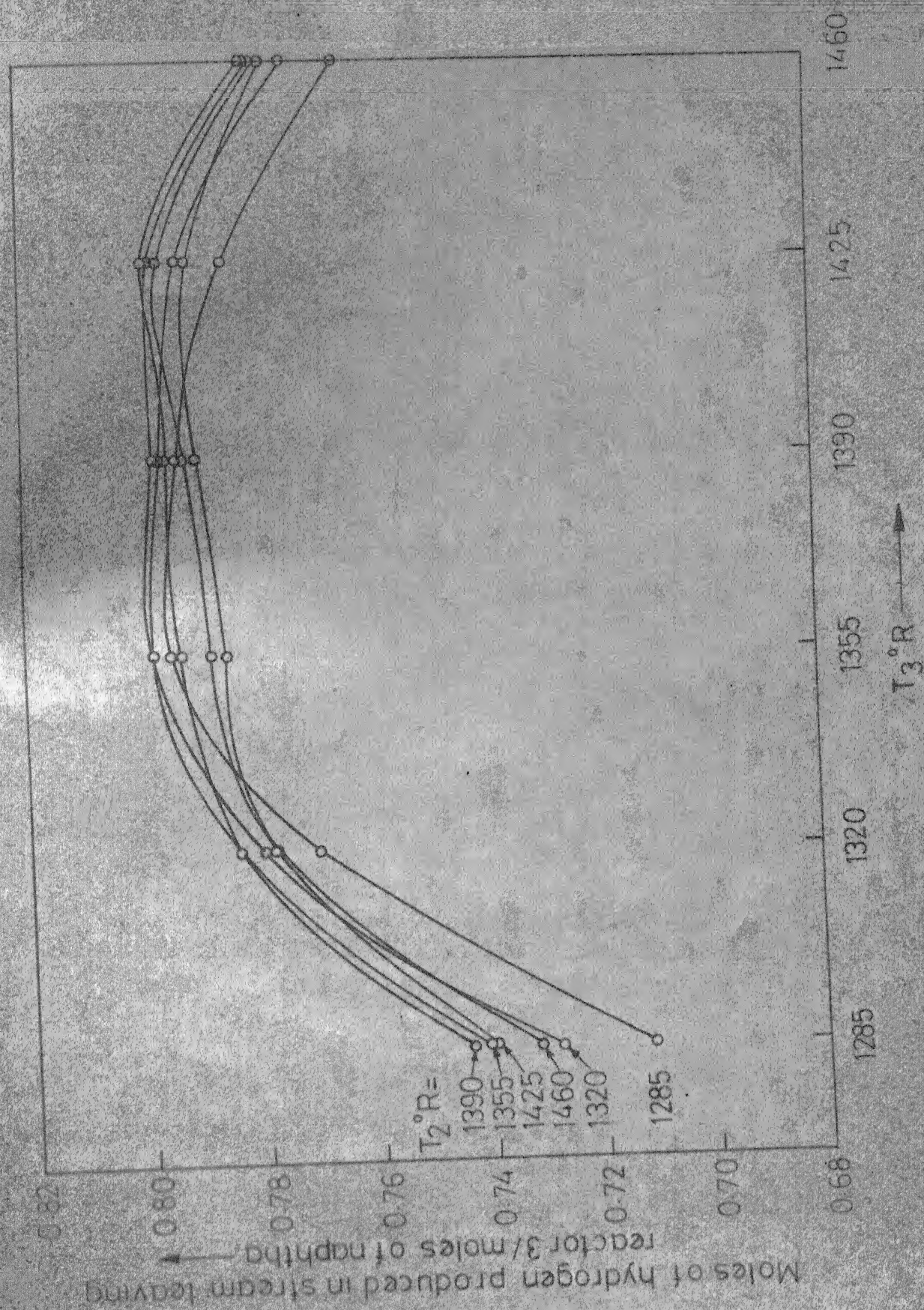


Fig 8 - Effect of temperature on conversion of hydrogen for $T_1 = 1460^\circ\text{R}$

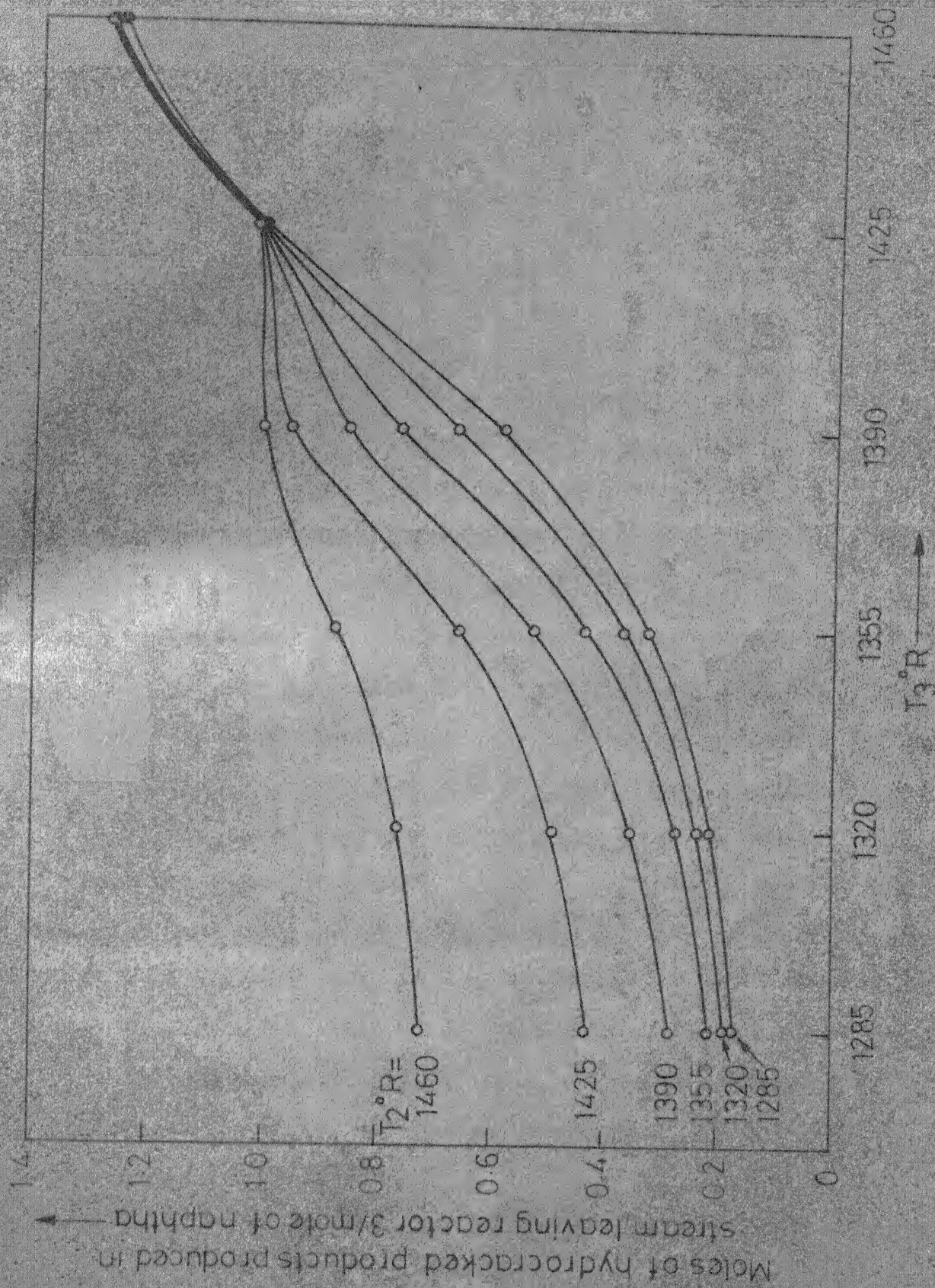


Fig. 9 - Effect of temperature on conversion of hydrocracked products for

the increase in aromatics production rate decreases. At higher recycle ratio, the effect of extra heat produced because of reaction (2.2) becoming fast to make the reaction (2.1) fast, decreases.

(ii) Effect of Pressure:

It can be seen from Figure 6 that as pressure of inlet stream rises from 17 to 27 atmospheres, the production of aromatics rises from .3985 to .4131 and then decreases from .4131 to .3431 moles of aromatics/mole of naphtha as pressure rises from 27 to 47 atmospheres. From the Le Chatellier's, principle one will expect the production of aromatics to go down with an increase in pressure, because both in naphthenes dehydrogenation to aromatics and paraffin dehydrogenation to naphthenes a rise in number of moles is resulted. As the pressure rises exothermic reaction (2.2) becomes fast and leads to a rise in the temperature of reaction mixture, and at high temperatures, the reaction (2.1) which is endothermic becomes fast enough to off set the decrease in the rate of dehydrogenation of naphthenes to aromatics because of increase in pressure. But as pressure rises, the rise in temperature because of (2.2) becoming fast is not sufficient enough to off-set the effect of the rise in pressure and as a result the production of aromatics goes down.

(iii) Effect of Temperature:

The effect of temperature on production of aromatics, hydrogen and hydrocracked product is given in Table II and figures 7, 8 and 9. Figures 7, 8 and 9 represent a typical set of curves for one inlet set of temperature for reactor-1. It can be seen from Table II that the amount of aromatics and hydrogen in the stream leaving reactor-1 is approximately a linear function of temperature. The amount of aromatics produced in reactor-2 is also approximately a linear function of T_2 for every value of T_1 . The amount of aromatics in the stream leaving the reactor-3 rises with rise in temperature of inlet stream to any reactor except for $T_1 > 1390$, $T_2 > 1355$ and 1425°R .

For the above excepted value a rise in inlet temperatures of all reactors, produces only marginal decrease in production of aromatics.

For $T_1 = 1425$ and $T_2 \geq 1390$, and $T_1 = 1460$ and $T_2 \geq 1355$ amount of aromatics is less in the stream leaving reactor-3 than the stream leaving reactor-2 for $T_3 = 1285$. At the above values of T_1 and T_2 , conversion of naphthenes to aromatics is very fast in reactor one and two. The concentration of naphthenes in reaction mixture of reactor-3 for $T_3 = 1285$ is low enough to reverse the direction of reaction (2.1) as this reaction is endothermic. Since reaction (2.2) is exothermic, at low temperature hydrogenation of naphthenes to paraffins is favoured and as a result the concentration of naphthenes is lowered.

It is seen from Fig. 7 that amount of aromatics produced at $T_1 = 1460$ and $T_3 = 1460$ is approximately independent of T_2 .

As hydrogen takes part in all the reactions, its production does not follow any pattern (See Figure 8).

The production of hydrocracked products rises with the rise in temperature of the inlet streams and it is seen from Figure 9 that it's amount is approximately independent of T_2 for $T_1 = 1460$ and T_3 between 1425 and 1460.

OPTIMIZATION:

The procedure outlined in Chapter IV to minimize an objective function, ϵ , with constraints on temperature and concentrations of the stream leaving the last reactor of the series was used to minimize the total weight of catalyst and operating cost for three, four and five reactors in series. The respective objective function for total weight of catalyst and operating cost, and the constraints are given in Appendix D. The results obtained by computer programme (see Appendix E) developed in the present study, are given in Table III and IV (For additional data, please see Appendix A).

When minimizing the total weight of catalyst and the operating cost for five reactors in series catalyst weight for one of these reactors come out to be zero. Though the

TABLE III: RESULTS FOR MINIMIZATION OF WEIGHT OF CATALYST

SS = Starting solution

FS = Final solution

		Reactor					Total wt. of cata- lyst lb.	
		1	2	3	4	5		
Three Reactors	SS	W _i	1500.0	1940.0	13900.0		17340.0	
		T _i	1378.8	1389.6	1398.6			
	FS	W _i	327.9	658.7	12437.1		13423.7	
		T _i	1402.3	1380.6	1439.5			
Four Reactors	SS	W _i	1500.0	1940.0	6900.0	6900.0	17340.0	
		T _i	1378.8	1389.6	1398.6	1375.0		
	FS	W _i	1215.9	1283.4	831.4	1387.0	4717.7	
		T _i	1402.9	1433.1	1460.0	1408.7		
Five Reactors	SS	W _i	1500.0	1940.0	4633.3	4633.3	4633.3	17340.0
		T _i	1378.8	1389.6	1398.6	1375.0	1374.0	
	FS	W _i	0.0	472.8	3241.7	3242.7	3263.8	10221.0
		T _i	1366.0	1366.0	1391.5	1438.9	1372.6	

TABLE IV: RESULTS FOR MINIMIZATION OF OPERATING COST

SS = Starting solution

FS = Final solution

		Reactor					Operating cost in lakhs of Rs. per year	
		1	2	3	4	5		
Three Reactor	SS	W_i	1500.0	1940.0	13900.0		32.36	
		T_i	1378.8	1389.6	1398.6			
	FS	W_i	1159.7	1459.8	12858.2		29.44	
		T_i	1367.7	1391.7	1410.3			
Four Reactor	SS	W_i	1500.0	1940.0	6900.0	6900.0	32.22	
		T_i	1378.8	1389.6	1398.6	1375.0		
	FS	W_i	1967.8	2036.2	1445.3	2336.6	17.75	
		T_i	1355.2	1373.0	1406.7	1429.3		
Five Reactor	SS	W_i	1500.0	1940.0	4633.3	4633.3	4633.3	32.39
		T_i	1378.8	1389.6	1398.6	1375.0	1374.0	
	FS	W_i	2298.7	2462.3	2302.1	0.0	1480.4	19.03
		T_i	1357.0	1375.0	1409.9	1360.6	1436.7	

three starting solutions which were tried led to one of W_i going to zero, there can be an initial solution which can avoid such a situation.

Since the iterations were stopped when one of the W_i values went to zero, the final solutions given in Tables III and IV for the five reactors in series do not represent the real optimum. When these values were used as a starting solution for the four reactors in series, approximately the same results were obtained as given in Tables III and IV for four reactor cases.

From the results obtained it is concluded that one should use four reactors in series. But the result can be different if one maximizes for venture profit. In operating cost the number of inter heaters, which depend on the number of reactors being used is not considered but will figure in venture profit.

During computation, it was found necessary to reduce the scale of temperature and naphtha feed rate by factors of 10-40 and 50-100 respectively. It was also found necessary to reduce the scale of optimization function by a factor of 100 when minimizing the operating cost. These scaling were made necessary for, in the development of algorithm, second and higher order terms have been assumed to be negligible as compared to the first order terms. In order to reduce the total

number of iterations, it was found useful to use a lower factor for temperature and a higher for naphtha feed rate initially and then keep changing these factors after some iterations.

The values of constraints g_1 and g_2 were .046 and .5731 respectively at the starting of the iterations for optimization in all the cases considered for the optimization study. These equality constraints were allowed only a change of $\pm .0005$ and $\pm .005$ respectively from the starting value. If the change in the values of g_1 and g_2 was more than the above given value, w^* , the multiplication factor to determine the magnitude of changes in decision variables, which had an initial value 4, was reduced to half each time till the constraints met the prescribed limits.

The iterations were stopped when changes in objective functions for the weight of catalyst and the operating cost were less than 1.0 and 50.0 respectively. For both the objective functions, the time taken on IBM 7044 to reach the final solution from the starting solution were approximately 20, 35 and 15 minutes respectively.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

The mathematical model developed for the catalytic-reforming process predicted very well the temperature and concentration of various components in the exit stream of the reactors, for two different industrial units.

Simulated results show that as recycle ratio rises, the production of aromatics also increases. Maximum production of aromatics occur at a pressure of 27 atmospheres. The rise in temperature of inlet stream increases the production of aromatics and hydrocracked products. From the simulated results, it is recommended that for the plant of Appendix A, the temperatures of inlet streams should be changed to $T_1 = 1390$, $T_2 = 1390$ and $T_3 = 1460$ from the existing values, to increase the production rate of aromatics to 135.2 moles/hr from its present value of 112.2. The increase in temperature will lead to more load on inter heaters. So one has to make an economic evaluation of the process before taking the final decision.

If one wishes to use the minimum weight of catalyst, or to have the minimum operating cost to produce aromatics at a rate, being produced in plant of Appendix A from naphtha (its composition and feed rate are given in Appendix A), one should use four reactors in series.

In the existing plant (Appendix A) one can use less weight of catalyst or operate at lower operating cost for the same aromatic production rate and the same quality of reformate. The weight of catalyst can be reduced by 19.8 per cent (See Table III) and operating cost by 9.05 per cent by changing, the catalyst distribution in the reactors and temperature of inlet streams to the reactors.

RECOMMENDATIONS FOR FURTHER STUDIES:

1. In the present study, inter heaters have not been included in the simulation. A mathematical model representing the behaviour of inter heaters can be combined with the present simulation model.
2. Mathematical model representing the flash unit can also be incorporated with the present simulation model.
3. Recycle ratio and operating pressure can also be used as variables in the optimization function.
4. For design optimization of Platformer unit, a venture profit concept can be used as an objective function.

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APPENDIX A

PLANT DATA FOR THREE REACTORS SET-UP

Feed = 272.2 moles/hr.

Recycle ratio = 7.95

Reactor	Weight of catalyst lb	Temp. of inlet stream °R	Pressure of inlet stream atm.
1	1500	1378.8	22.0
2	1940	1389.6	20.5
3	13900	1398.6	18.6

Naphtha Feed Composition:

C ₇ -Paraffins	2.2 % by wt.
C ₇ -Naphthenes	2.9 "
C ₇ -Aromatics	2.0 "
C ₈ -Paraffins	29.0 "
C ₈ -Naphthenes	29.3 "
C ₈ -Aromatics	12.6 "
C ₉ -Paraffins	18.4 "
C ₉ -Naphthenes	3.6 "

Recycle Gas Composition:

Hydrogen	86.0	Mole %
Methane	6.0	"
Ethane	2.8	"
Propane	2.1	"
Butane	1.0	"
Pentane	0.5	"
C ₆ -Paraffins	0.6	"
C ₆ -C ₈ Hydrocarbons	1.0	"

APPENDIX B

PLANT DATA FOR FOUR REACTORS SET-UP

Feed = 232.8 moles/hr

Recycle ratio = 6.9

Reactor	Weight of catalyst lb	Temperature of inlet stream °R	Pressure of inlet stream atm.
1	1180	1403	39.9
2	1180	1403	39.5
3	3230	1403	39.1
4	4150	1403	38.1

Naphtha feed composition:

C ₆ -Paraffins	0.3 % by wt.
C ₆ -Naphthenes	0.7 "
C ₆ -Aromatics	0.1 "
C ₇ -Paraffins	5.9 "
C ₇ -Naphthenes	9.3 "
C ₇ -Aromatics	3.7 "
C ₈ -Paraffins	23.9 "
C ₈ -Naphthenes	26.1 "
C ₈ -Aromatics	11.5 "
C ₉ -Paraffins	15.0 "
C ₉ -Naphthenes	1.9 "
C ₉ -Aromatics	1.6 "

Recycle Gas Composition:

Hydrogen	86.4	Mole %
Methane	5.1	"
Ethane	3.6	"
Propane	2.1	"
Butane	1.406	"
Pentane	0.666	"
Hexane and higher	0.698	"

APPENDIX C

HEAT CAPACITIES

Let it be assumed that $SP1_i + SP2_i.T$, $SN1_i + SN2_i.T$, $SA1_i + SA2_i.T$, $SH1 + SH2.T$ are specific heats and; XP_i , XN_i , XA_i , XH_i are mole fractions of, paraffins, naphthenes, aromatics and hydrogen in the feed to first reactor where 'i' is number of carbon atoms. And since C_{10} and higher compounds are negligible, the specific heat for various classes of compounds in the feed to first reactor e.g., C_6 and higher paraffins, naphthenes, aromatics and C_5 and lower paraffins, hydrogen and hydrocarbons produced from hydrocracking, can be written as:

$$C_{pP} = \frac{\sum_{i=6}^9 SP1_i \cdot XP_i}{\sum_{j=6}^9 XP_j} + \frac{\sum_{i=6}^9 SP2_i \cdot XP_i}{\sum_{i=6}^9 XP_i} \cdot T$$

$$C_{pN} = \frac{\sum_{i=6}^9 SN1_i \cdot XN_i}{\sum_{i=6}^9 XN_i} + \frac{\sum_{i=6}^9 SN2_i \cdot XN_i}{\sum_{i=6}^9 XN_i} \cdot T$$

$$C_{pA} = \frac{\sum_{i=6}^9 SA1_i \cdot XA_i}{\sum_{i=6}^9 XA_i} + \frac{\sum_{i=6}^9 SA2_i \cdot XA_i}{\sum_{i=6}^9 XA_i} \cdot T$$

$$C_{pHCl} = \frac{\sum_{i=1}^5 SP1_i \cdot XP_i}{\sum_{i=1}^5 XP_i} + \frac{\sum_{i=1}^5 SP2_i \cdot XP_i}{\sum_{i=1}^5 XP_i} \cdot T$$

$$C_{pH} = SH1 + SH2 \cdot T$$

$$C_{pHC} = \frac{1}{5} \sum_{i=1}^5 SP1_i + \frac{1}{5} \sum_{i=1}^5 SP2_i \cdot T$$

Values of $SP1_i$, $SP2_i$, $SA1_i$, $SA2_i$, $SH1$ and $SH2$ for the catalytic reforming temperature conditions are given below (1)

$$SH1 = 4.02$$

$$SH2 = .00024$$

i	SP1 _i	SP2 _i	SN1 _i	SN2 _i	SA1 _i	SA2 _i
1	5.34	.00678				
2	8.97	.0117				
3	13.30	.016				
4	18.77	.0222				
5	23.53	.02492				
6	28.28	.0292	21.48	.02958	18.55	.0184
7	32.98	.0326	25.62	.0344	23.57	.023
8	37.86	.038	30.50	.0388	28.18	.027
9	42.53	.0424	35.07	.0432	33.5	.0311

References:

1. American Petroleum Institute, Research Project 44.

APPENDIX D

OBJECTIVE FUNCTIONS AND CONSTRAINTS

1. Objective function for total weight of catalyst:

$$= W_1 + W_2 + \dots W_N$$

2. Objective function for operating cost:

$$= \frac{(\text{Wt. of catalyst (lb)})(\text{Cost of catalyst (Rs/lb)})}{\text{Life of catalyst (Yrs.)}}$$

$$+ \text{heat duty (Btu/yr)} \cdot \text{heating cost (Rs./Btu)}$$

$$+ F_T \cdot \text{pumping cost (Rs./Yr. lb mole /hr.)}$$

$$\text{Cost of catalyst (1)} = 140 \text{ Rs/lb.}$$

$$\text{Life of catalyst (1)} = .9 \text{ years}$$

$$\text{Pumping cost (2)}$$

$$= 38.2 ((\text{pressure of stream entering the first reactor of the series/pressure of stream leaving the last reactor of the series})^{.286} - 1.0) \text{ Rs/(yr. lb m/hr)}$$

$$\text{Heating cost (2)} = 390.0 \text{ Rs./million Btu}$$

3. Constraints:

$$1. \quad g_1 = X_{N1} (W_N)$$

$$2. \quad g_2 = \text{Concentration of aromatics in the reformat leaving flash unit}$$

$$= \frac{\text{Moles of aromatics in reformat}}{\text{Moles of reformat}}$$

It can be seen from the recycle gas composition that moles of C_5 and higher hydrocarbons in recycle gas are approximately .0134 moles per mole of hydrogen. Assuming that whole of the hydrogen is separated in the flash unit, it can be said that .0134 mole of hydrocarbons/mole of hydrogen produced are separated in flash unit along with hydrogen. Thus,

$$\begin{aligned}
 \text{Moles of reformat per mole } F_T &= X_{AI} + X_{NI} + X_{PI} \\
 &- X_{N3}(w_N) - X_{N4}(w_N) - .0134 (3X_{N1}(w_N) - X_{N2}(w_N)) \\
 &- \frac{n}{15} X_{N3}(w_N) - \frac{n}{15} X_{N4}(w_N)) \\
 g_2 &= (X_{AI} + X_{N1}(w_N)) / (X_{AI} + X_{NI} + X_{PI} - .0134 \cdot 3X_{N1}(w_N) \\
 &+ .0134 X_{N2}(w_N) + (.0134 \frac{n-3}{3} - \frac{15-n}{15}) X_{N3}(w_N) \\
 &+ (.0134 \frac{n}{3} - \frac{15-n}{15}))
 \end{aligned}$$

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APPENDIX E

JOB CCG136,TIME 8,PAGES 37,NAME ASHOK KUMAR SHARMA

IBJOB

IBFTC MAIN

SIMULATION PROGRAMME

THIS PROGRAMME IS TO PREDICT THE OUT PUT STREAMS FROM EACH REACTOR FOR GIVEN RECYCLE GAS FLOW RATE, NAPHTHA FEED RATE, TEMPERATURES AND PRESSURES FOR INLET STREAM TO EACH REACTOR AND WEIGHT OF CATALYST IN EACH REACTOR

IR IS NUMBER OF REACTORS IN SERIES

FEED AND RECY ARE LB MOLES OF NAPHTHA FEED AND RECYCLE GAS PER HOUR

PP IS PRESSURE OF THE INLET STREAM TO VARIOUS REACTORS

TT AND WC ARE TEMPERATURES OF INLET STREAMS AND WEIGHT OF CATALYST IN EACH REACTOR

C6PINR IS MOLE FRACTION OF C6 AND HIGHER HYDROCARBONS IN RECYCLE GAS

INC IS NUMBER OF PARTS IN WHICH A REACTOR IS DEVIDED FOR INTEGRATION

DATA CARDS

MOLE FRACTIONS OF RECYCLE GAS COMPONENTS STARTING FROM METHANE TO HEXANE AND HYDROGEN IN 1.F8.4 FORMAT

WEIGHT PERCENTAGES OF PARAFFINS(C6 TO C9), NAPHTHENES(C6 TO C9) AND AND AROMATICS(C6 TO C9) IN 1.F8.4 FORMAT

NUMBER OF REACTORS (I6)

TEMPERATURE VECTOR,WEIGHT OF CATALYST VECTOR AND PRESSURE VECTOR (8F10.1)

MOLE FRACTICHS OF C6 AND HIGHER COMPONENTS IN RECYCLE GAS (10F8.4)

FEED AND RECY (8F10.1)

REAL MWF,MWRB,N

DIMENSION AAA(7),AAH(7),AAHC(7)

DIMENSION CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)

DIMENSION TT(4),PP(4)

COMMON /BL1/ X1,X2,X3,X4,TI,XAI,XPI,XNI,XHI,XHYI,AC

COMMON /BL2/ IJ,TT,AB

COMMON /BL3/ A1,A2,AB,A4,P,FT,N

COMMON /BL4/ AD(2,5)

COMMON /BL6/ C(3),F

COMMON /BL8/ INC

DIMENSION WC(4)

CALL CPEV

C(1)=2.

C(2)=2.

C(3)=1.

FT=FEED+RECY

READ 60,IR

READ 61,(TT(I),WC(I),PP(I),I=1,IR)

FORMAT(I6)

FORMAT(8F10.1)

READ 61,FEED,RECY

READ 61,C6PINR

XAI=XAF*CONV+RECY*C6PINR/FT

```

INC=6
DO 10 I=1,2
  A0=CPA(I)*XAI+CPP(I)*XPI+CPN(I)*XNI+CPH(I)*XHI+CPHYI(I)*XHYI
  A1=CPA(I)-CPN(I)+2.*CPH(I)
  A2=CPP(I)-CPN(I)-CPH(I)
  A3=CPHYI(I)*N/3.-CPP(I)-(N-3.)*CPH(I)/3.
  A4=CPHYI(I)*N/3.-CPN(I)-CPH(I)*N/3.
  AD(I,1)=A0
  AD(I,2)=A1
  AD(I,3)=A2
  AD(I,4)=A3
  AD(I,5)=A4
10 CONTINUE
  AB=FT/272.2
  PRINT14
14 FORMAT(////1X,*REACTOR WT CATA T IN R T OUT R AROMAT NAPHTH
1 PARAFFIN H2 HYDROC*//)
  X1=0.
  X2=0.
  X3=0.
  X4=0.
  DO 1 I=1,IR
    TI=TT(I)
    H=WC(I)/FLCAT(INC)
    P=PP(I)
    CALL SIMULA
    AA=(XAI+X1)*FT
    AP=(XPI+X2-X3)*FT
    AH=(XHI+3.*X1-X2-(N-3.)*X3/3.-N*X4/3.)*FT
    AN=(XNI-X1-X2-X4)*FT
    AHY=(XHYI+(X3+X4)*N/3.)*FT
    PRINT13,I,WC(I),TI,TT(I),TI,AA,AN,AP,AH,AHY
13 FORMAT(1X,I4,F12.1,F8.1,F9.1,F7.1,F8.1,F9.1,F10.1,F8.1/)
1 CONTINUE
  STOP
  END
IBFTC SUB1
SUBROUTINE SIMULA
C
C THIS SUBROUTINE IS TO SIMULATE THE REACTORS
C
REAL N,K(4,5)
DIMENSION PHI(5)
DIMENSION TT(4)
COMMON /BL1/ X1,X2,X3,X4,TI,XAI,XPI,XNI,XHI,XHYI,A0
COMMON /BL2/ J,TT,AB
COMMON /BL3/ A1,A2,A3,A4,P,FT,N
COMMON /BL4/ AD(2,5)
COMMON /BL6/ C(3),H
COMMON /BL8/ INC
A11(T)=EXP(23.21-34750./T)
A21(T)=EXP(46.15-46145./T)
A12(T)=EXP(35.98-59600./T)
A22(T)=EXP(8000./T-7.12)
A31(T)=EXP(42.97-62300./T)

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XNI=XNF*FEED/FT
XPI=XPF*FEED/FT
XHYI=XHYR*RECY/FT-RECY*C6PINR/FT
XHI=XH2R*RECY/FT
N=(MWF-2.*XNF+6.*XAF)/14.
F1(P)=C1*P*(XN-P**3*XA*XH**3/(E2*A**3))/(FT*A)
F2(P)=E3*P*(P*XN*XH/E-XP/E4)/(FT*A)
F3(A)=E5*XP/(FT*A)
F4(A)=E5*XN/(FT*A)
F5(C1)=(-C1*91000.*+19000.*C2+(N-3.)*81000.*C3+N*223000.*C4/3.)/CP
DO 1 I=1,INC
T=TI
X1C=X1
X2C=X2
X3C=X3
X4C=X4
DO 2 I=1,4
A=1.+3.*X1C-X2C-X4C
XA=XAI+X1C
XP=XPI+X2C-X3C
XH=XHI+3.*X1C-X2C-(N-3.)*X3C/5.-N/3.*X4C
XN=XNI-(X1C+X2C+X4C)
F1=A11(T)
F2=A21(T)
F3=A12(T)
F4=A22(T)
F5=A31(T)
C1=F1(P)
C2=F2(P)
C3=F3(A)
C4=F4(A)
A0=AD(1,1)*T+AD(2,1)
A1=AD(1,2)*T+AD(2,2)
A2=AD(1,3)*T+AD(2,3)
A3=AD(1,4)*T+AD(2,4)
A4=AD(1,5)*T+AD(2,5)
CP=A0+A1*X1C+A2*X2C+A3*X3C+A4*X4C
K(I,1)=C1
K(I,2)=C2
K(I,3)=C3
K(I,4)=C4
K(I,5)=F5(C1)
IF(I.EQ.4) GO TO 2
X1C=X1+H*K(I,1)/C(1)
X2C=X2+H*K(I,2)/C(1)
X3C=X3+H*K(I,3)/C(1)
X4C=X4+H*K(I,4)/C(1)
T=TI+H*K(I,5)/C(1)
2 CONTINUE
DO 3 I=1,5
PHI(I)=(K(1,I)+2.*K(2,I)+2.*K(3,I)+K(4,I))/6.
X1=X1+H*PHI(1)
X2=X2+H*PHI(2)
X3=X3+H*PHI(3)
X4=X4+H*PHI(4)

```

```

      TI=TI+H*PHI(F)
4     FORMAT(/IX,I4,9F10.4,F10.1)
      CONTINUE
      RETURN
      END
IBFTC SUB2
      SUBROUTINE CPEV
      COMMON /BL15/ CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
      COMMON /BL16/ XPF,XNF,XAF,XHYR,XH2R,MWF,MWRE
      DIMENSION WCR(7),WCP(4),WCN(4),WCA(4),CP(2,10),CN(2,4),CA(2,4)
      REAL MCR(7),MCP(4),MCN(4),MCA(4),M
      REAL MWF,MWRE
      DATA CP/38.88,15.1,23.72,25.83,34.20,37.8,44.55,48.23,54.33,59.30,65.10 7
1,65.10,7.36,75.38,81.43,85.60,92.50,95.93,103.56,7.035,7.078/
      DATA CN/58.68,54.0,69.2,75.22,79.30,86.28,89.57,97.35/
      DATA CA/41.70,45.6,51.57,55.72,62.28,67.15,72.70,78.3/
      READ2,WCR
      READ2,WCP,WCN,WCA
2     FORMAT(1,F8.4)
      A=2.
      B=0.
      DO 8 I=1,6
      MCR(I)=WCR(I)/1.0.
      A=A+14.
8     B=B+MCR(I)*A
      MCR(7)=WCR(7)/1.0.
      MWRE=B+MCR(7)*2.
      XHYR=1.-MCR(7)
      XH2R=MCR(7)
      AA=72.
      XAF=0.
      XNF=0.
      XPF=0.
      DO 1 I=1,4
      AA=AA+14.
      BB=AA-2.
      CC=AA-8.
      MCP(I)=WCP(I)/AA
      MCN(I)=WCN(I)/BB
      MCA(I)=WCA(I)/CC
      XPF=XPF+MCP(I)
      XNF=XNF+MCN(I)
1     XAF=XAF+MCA(I)
      A=XPF+XNF+XAF
      MWF=100./A
      XPF=XPF/A
      XNF=XNF/A
      XAF=XAF/A
      DO 4 I=1,4
      MCP(I)=MCP(I)/A
      MCN(I)=MCN(I)/A
4     MCA(I)=MCA(I)/A
      A=0.
      B=0.
      D=0.

```

```

DD=0.
DO 5 I=1,6
M=-(CP(1,I)-CP(2,I))/10.
C=CP(1,I)-M*7.
D=D+M
DD=DD+C
A=A+M*MCR(I)
5 B=B+C*MCR(I)
CPHYI(1)=A/XHYR
CPHYI(2)=B/XHYR
M=-(CP(1,10)-CP(2,10))/10.
CPH(1)=M
CPH(2)=CP(1,10)-M*7.
CPHY(1)=D/5.
CPHY(2)=DD/5.
A=0.
B=0.
D=0.
AA=0.
BB=0.
DD=0.
DO 6 I=1,4
J=I+5
M=-(CP(1,J)-CP(2,J))/10.
C=CP(1,J)-M*7.
A=A+M*MCP(I)
AA=AA+C*MCP(I)
M=-(CN(1,I)-CN(2,I))/10.
C=CN(1,I)-M*7.
B=B+M*MCN(I)
BB=BB+C*MCN(I)
M=-(CA(1,I)-CA(2,I))/10.
C=CA(1,I)-M*7.
6 D=D+M*MCA(I)
DD=DD+C*MCA(I)
CPP(1)=A/XPF
CPP(2)=AA/XPF
CPN(1)=B/XNF
CPN(2)=BB/XNF
CPA(1)=D/XAF
CPA(2)=DD/XAF
CPP(1)=CPP(1)/1.8
CPN(1)=CPN(1)/1.8
CPA(1)=CPA(1)/1.8
CPH(1)=CPH(1)/1.8
CPHY(1)=CPHY(1)/1.8
CPHYI(1)=CPHYI(1)/1.8
RETURN
END

```

ENTRY

JOB CGG136,TIME03,PAGES00,NAME ASHOK KUMAR SHARMA

IBJOB

IBFTC MAIN

PROGRAMME FOR MINIMIZATION OF WEIGHT OF CATALYST

IR IS NUMBER OF REACTORS IN SERIES

FEED AND RECY ARE LB MOL% OF NAPHTHA FEED AND RECYCLE GAS PER HOUR

PP IS PRESSURE OF THE INLET STREAM TO VARIOUS REACTORS

TT AND WC ARE TEMPERATURES OF INLET STREAMS AND WEIGHT OF CATALYST IN EACH REACTOR

INC IS NUMBER OF PARTS IN WHICH A REACTOR IS DIVIDED FOR INTEGRATION

C6PINR IS MOLE FRACTION OF C6 AND HIGHER HYDROCARBONS IN RECYCLE GAS

AB1 IS NUMBER OF MOLES OF NAPHTHA WHICH ARE USED AS BASIS OF CALCULATIONS FOR OPTIMIZATION

ABC IS SCALING FACTOR FOR TEMPERATURE

VALUES OF AB1 AND ABC ARE CHANGED DURING ITERATIONS AT SUITABLE PLACES

THOUGH THE GIVEN STARTING VALUES HAVE BEEN FOUND TO BE GOOD, BUT IT IS

ADVISED TO TRY OTHER STARTING VALUES FOR THESE FACTORS TO MINIMIZE TOTAL NUMBER OF ITERATIONS

DIV IS A FACTOR TO DECIDE MAGNITUDE OF CHANGES IN DECISION VARIABLES

SO THAT ALL THE CONSTRAINTS ARE SATISFIED

ITR3 IS MAXIMUM NUMBER OF ITERATIONS FOR WHICH THE PROGRAMME IS ALLOWED TO EXECUTE

ER1 AND ER2 ARE AMOUNTS OF ERRORS ALLOWED IN CONSTRAINTS ONE AND TWO ON THE FINAL PRODUCT STREAM

ER, IF THE CHANGE IN OBJECTIVE FUNCTION IS LESS THAN ER PROGRAMME IS

TERMINATED AUTOMATICALLY AND THE SOLUTION VECTOR AT THIS PLACE IS PRINTED AS OPTIMIZED RESULTS

IT IS ADVISED THAT MANY INITIAL SOLUTIONS BE TRIED TO ENSURE THE VALIDITY OF THE RESULTS

DATA CARDS

MOLE FRACTIONS OF RECYCLE GAS COMPONENTS STARTING FROM METHANE TO HEXANE AND HYDROGEN IN 10F8.4 FORMAT

WEIGHT PERCENTAGES OF PARAFFINS(C6 TO C9), NAPHTHENES(C6 TO C9) AND AROMATICS(C6 TO C9) IN 10F8.4 FORMAT

NUMBER OF REACTORS (I6)

TEMPERATURE VECTOR, WEIGHT OF CATALYST VECTOR AND PRESSURE VECTOR (8F10.0)

MOLE FRACTIONS OF C6 AND HIGHER COMPONENTS IN RECYCLE GAS (10F8.4)

FEED AND RECY (8F10.0)

THESE TT AND WC VALUES ARE USED AS A STARTING VECTOR FOR OPTIMIZATION

AT THESE VALUES ALL THE CONSTRAINTS SHOULD BE SATISFIED

COMMON /BL1/ X1,X2,X3,X4

COMMON /BL3/ A1,A2,A3,A4,P,FT

COMMON /BL6/ C(3),H

COMMON /BL7/ IJ,FU(5,5)

COMMON /BL8/ INC,INC1,INC2

COMMON /BL9/ ABC

COMMON /BL10/ N

COMMON /BL11/ CD(4),C1,C2,B1,B2,B3,DIV,IR,IR1

COMMON /BL12/ TI,XAI,XPI,XNI,XHI,XHYI,AU

COMMON /BL13/ TIN(5),WIN(5)

COMMON /BL14/ WC,A

```

COMMON /BL15/ CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
COMMON /BL16/ XPF,XNF,XAF,XHYR,XH2R,MWF,MWRE
COMMON /BL17/ AD(2,5)
DIMENSION PP(5),WC(5),TT(5)
DIMENSION AA(5,3),AAA(5,8),PT(5),PW(5)
DIMENSION ABD(5),AC2(3)
REAL M,MWF,MWRE
DATA PT,PW/6H T1 ,6H T2 ,6H T3 ,6H T4 ,6H T5 ,6H W1 ,
16H W2 ,6H W3 ,6H W4 ,6H W5 /
FR=1.
CALL CP4V
FRI=.5
FR2=.5
WC2=1.5+3.5
IC4=
AB1=1.1
ABC=2.0
DIV=1.
DIV1=DIV
READ61,IR
READ 61,(TT(I),WC(I),PP(I),I=1,IR)
60 FORMAT(I6)
61 FORMAT(8F10.0)
IR1=IR-1
IT5=0
C(1)=2.
C(2)=2.
C(3)=1.
READ61,FEED,RECY
READ61,C6PINR
AFT=FEED+RECY
A=FEED
DO 18 I=1,IR
18 WC(I)=WC(I)*AB1/A
PRINT3
3 FORMAT(1H1)
2 FORMAT(///1X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,30X,*FEED DATA*,30
1X,1H*/10X,1H*,70X,1H*/10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,70X,1H*)
PRINT17,FEED,RECY,MWF,MWRE
17 FORMAT(1X,1H*,20X,*NAPHTHA FEED LB MOLE/HR =*,F8.1,17X,1H*/10X,1H
1*,70X,1H*/10X,1H*,21X,*RECYCLE GAS LB MOLE/HR =*,F8.1,17X,1H*/10X,
21H*,70X,1H*/10X,1H*,17X,*LB MOLECULAR WT OF NAPHTHA =*,F8.1,17X,1H
3*/10X,1H*,70X,1H*/10X,1H*,13X,*LB MOLECULAR WT OF RECYCLE GAS =*,F
48.1,17X,1H*/10X,1H*,70X,1H*)
CD(1)=XAF*FEED+RECY*C6PINR
DD(2)=XNF*FEED
DD(3)=XPF*FEED
DD(4)=XHYR*RECY-RECY*C6PINR
A=XH2R*RECY
PRINT19,DD,A,PP(1)
19 FORMAT(10X,1H*,23X,*AROMATICS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,7
10X,1H*/10X,1H*22X,*NAPHTHENES LB MOLE/HR =*,F8.1,17X1H*/10X1H*70X1
2H*/10X1H*23X*PARAFFINS LB MOLE/HR =*F8.1,17X,1H*/10X,1H*,70X,1H*/1
30X,1H*,2X,*HYDROCARBONS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,70X,1H

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4*,/10X,1H*,24X,*HYDROGEN LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*70X,1H*
5/10X,1H*,22X,*INLET PRESSURE (ATM) =*,F8.1,17X,1H*/10X,1H*,70X,1H*
6/10X,1H*,71X,1H*/10X,1H*,72(1H*))
FT=FEED+RECY
CONV=FEED/(FEED+RECY)
XAI=XAF*CONV+RECY*CAPINR/FT
XPI=XPF*CONV
XNI=XNF*CONV
XHI=XH2R*RECY/FT
XHYI=XHYR*RECY/FT-RECY*CAPINR/FT
A=FEED
FT=AB1+RECY*AB1/A
N=(MWF-2.*XNF+6.*XAF)/14.
PRINT22,(PT(I),I=1,JP),(PW(I),I=1,IR)
PRINT6.2
22  FORMAT(1H1/10X,*ITER *,A6,9(2X,A6)/)
62  FORMAT(95X,6X,*C1*,8X,*C2*,4X,*OBJECTIVE FUNC*)
INC=50
INC1=INC+1
INC2=INC/2
XN=XNI
XP=XPI
XH=XHI
XA=XAI
DO 31 I=1,2
A0=CPA(I)*XA+CPP(I)*XP+CPN(I)*XN+CPH(I)*XH+CPHYI(I)*XHYI
A1=CPA(I)-CPN(I)+3.*CPH(I)
A2=CPP(I)-CPN(I)-CPH(I)
A3=CPHYI(I)*N/3.-CPP(I)-(N-3.)*CPH(I)/3.
A4=CPHYI(I)*N/3.-CPN(I)-CPH(I)*N/3.
AD(I,1)=A0
AD(I,2)=A1
AD(I,3)=A2
AD(I,4)=A3
AD(I,5)=A4
31  CONTINUE
DO 26 ITR4=1,ITR3
X1=0.
X2=0.
X3=0.
X4=0.
REWIND 1
DO 5 IJ=1,IR
P=PP(IJ)
TI=TT(IJ)
H=WC(IJ)/FLCAT(INC)
AA(IJ,1)=WC(IJ)*FEED/AB1
AA(IJ,2)=TI
CALL SIMULA
AA(IJ,3)=TI
AA(IJ,4)=AFT*(X1+XA)
AA(IJ,5)=AFT*(XNI-(X1+X2+X4))
AA(IJ,6)=AFT*(XP+X2-X3)
AA(IJ,7)=AFT*(XH+3.*X1-X2-(N-3.)*X3/3.-N*X4/3.)
AA(IJ,8)=AFT*(XHYI+(X3+X4)*N/3.)

```

```

5  CONTINUE
   IF(ITR4.EQ.1) C1=X1
   B1=XAI
   B2=XAI+XNI+XPI
   B3=.134
   A=B2-X1+B3*B3+X2*B3+X3*(B3*(N-3.)/3.-(15.-N)/15.)+X4*(B3*N/3.-(15.*N)
1-N)/15.)
   CD2=(B1+X1)/A
   IF(ITR4.EQ.1) C2=CD2
   PRINT22, ITR4, (TT(IJ), IJ=1, IR), (AA(IJ,1), IJ=1, IR)
23  FORMAT(10X, I3, 2F8.1)
   PRINT4, X1, CD2
40  FORMAT(10X, 2F10.4)
   DD(1)=1.+2.*B3*C2
   DD(2)=-B3*C2
   DD(3)=C2*(15.-N)/15.-B3*C2*(N-3.)/3.
   DD(4)=C2*(15.-N)/15.-B3*C2*(N-3.)/3.
   DD(1)=C2*A+(B1+X1)*(DD(1)-1.)
   DD(2)=DD(2)*(B1+X1)
   DD(3)=DD(3)*(B1+X1)
   DD(4)=DD(4)*(B1+X1)
   IF(ABS(C2-CC2).GT.EP2) GO TO 6
   IF(ABS(X1-C1).GT.EP1) GO TO 6
   IF(IT5.EQ.1) GO TO 1
   IF(ITR4.EQ. ITR3) GO TO 34
   DIV=DIV1
   CALL OPT1(IT, ICR)
   IF(IC3.EQ.0) GO TO 27
   D2=CD2
   D1=X1
   DWC=0.
   DO 43 IJ=1, IR
43  DWC=DWC+WIN(IJ)
   IF(DWC.LT.EC) GO TO 42
   IC4=1
   DIV=DIV1
   PRINT7
7  FORMAT(10X, *FOUND +VE*)
   AB1=AB1+.1
   ABC=ABC+2.
   DO 44 IJ=1, IR
44  WC(IJ)=AA(IJ,1)*AB1/FEED
   FT=AB1+RECY*AB1/FEED
   GO TO 24
42  DO 16 IJ=1, IR
   DO 16 I=1, 6
16  AAA(IJ,1)=AA(IJ,1)
   IC4=
   GO TO 41
6  PRINT8
8  FORMAT(10X, *CONST VIOLATED*)
   IT5=1
   DIV=DIV*2.
   DO 45 IJ=1, IR
   TT(IJ)=AAA(IJ,2)

```

```

45 WC(IJ)=AAA(IJ,.)*AB1/FRED
41 DO 35 IJ=1,IR
   ABD(IJ)=1.
   TIC=TT(IJ)+TIN(IJ)*ABC/DIV
   IF(TIC.GT.146.) GO TO 36
   IF(TIC.LT.126.) GO TO 37
   GO TO 35
36 ABD(IJ)=(146.-TIC)*DIV/(TIN(IJ)*ABC)
   AC2(IJ)=146.
   GO TO 35
37 ABD(IJ)=(126.-TIC)*DIV/(TIN(IJ)*ABC)
   AC2(IJ)=126.
35 CONTINUE
   IC1=1.
   DO 38 IJ=1,IR
   IF(ABD(IJ).LT.ABD(IC1)) IC1=IJ
38 CONTINUE
   AB3=ABD(IC1)
   WC1= .
   IT1=
   AC1=.
   DO 39 IJ=1,IR
   TT(IJ)=TT(IJ)+TIN(IJ)*AB3*ABC/DIV
   WC(IJ)=WC(IJ)+WIN(IJ)*AB3/DIV
   WC1=WC1+WIN(IJ)*AB3/DIV
   IF(WC(IJ).GT.(.)) GO TO 39
   IF(AC1.GT.WC(IJ)) IT1=IJ
39 CONTINUE
   IF(AB3.LT.1.) TT(IC1)=AC2(IC1)
   WC1=WC1*FRED/AB1
   WC1=-WC1
   IF(WC1.LT.8R) GO TO 10
   IF(IT1.EQ.0) GO TO 26
   AB4=WC(IT1)/(WIN(IT1)*AB3/DIV)
   DO 46 IJ=1,IR
   TT(IJ)=TT(IJ)-TIN(IJ)*AB3*AB4*ABC/DIV
46 WC(IJ)=WC(IJ)-WIN(IJ)*AB3*AB4/DIV
   ITE=1
26 CONTINUE
34 PRINT3
33 FORMAT(//1X,*ITERATION LESS FEED PROGRAMME AGAIN*//)
   GO TO 1
27 PRINT28
28 FORMAT(//5X,*LESS THAN TWO TEMPERATUTE ARE AWAY FROM BOUNDARY*//)
   GO TO 1
20 CONTINUE
DO 9 IJ=1,IR
DO 9 I=1,8
9 AA(IJ,I)=AAA(IJ,I)
X1=D1
CO2=D2
GO TO 10
10 PRINT21
21 FORMAT(1H1,5X,* OPTIMIZED RESULTS ARE*)
PRINT14

```

```

14  FORMAT(////1 X,*REACTOR WT CATA T IN R T OUT R AROMAT NAPHTH
1  PARAFFIN H2 HYDROG*//)
DO 12 I=1,IR
PRINT13,I,(AA(I,J),J=1,6)
13  FORMAT(1 X,I4,F12.1,F8.1,F9.1,F7.1,F8.1,F9.1,F10.1,F8.1/)
12  CONTINUE
PRINT15,C03
15  FORMAT(//1 X,*PERCENTAGE OF AROMATICS IN C5+ AT CUTLET=*,F6.3//)
STOP
END

```

IBFTC SUB1

SUBROUTINE SIMULA

C
C
C
C

THIS SUBROUTINE SIMULATE THE REACTOR AND PUT THE DERIVATIVES OF MODEL EQUA-
TIONS ON TAPE UNIT 1

```

COMMON /BL1/ X1,X2,X3,X4
COMMON /BL2/ E1,E2,E3,F4,E5,A,XA,XN,XP,XH,IC,CP,C1,C2,C3,C4,T
COMMON /BL3/ A1,A2,A3,A4,P,FT
COMMON /BL4/ D
COMMON /BL6/ C(3),F
COMMON /BL7/ IJ,FU(5,5)
COMMON /BL8/ INC,INC1,INC2
COMMON /BL9/ ABC
COMMON /BL10/ N
COMMON /BL11/ TI,XAI,XPI,XNI,XHI,XHYI,AC
COMMON /BL17/ AD(2,5)
DIMENSION D(5,5,51),PHI(5)
REAL N,K(4,5)
A11(T)=EXP(23.01-3475./T)
A21(T)=EXP(46.15-46045./T)
A12(T)=EXP(25.98-59600./T)
A22(T)=EXP(3700./T-7.12)
A31(T)=EXP(42.97-62300./T)
F1(P)=E1+P*(XN-P**3*XA*XH**3/(E2*A**3))/(FT*A)
F2(P)=E3+P*(P*XN*XH/A-XP/E4)/(FT*A)
F3(A)=E5*XP/(FT*A)
F4(A)=E5*XN/(FT*A)
F5(C1)=(-C1*91500.+19000.*C2+(N-3.)*8100.*C3+N*22300.*C4/3.)/CP
IC=0
DO 1 II=1,INC
T=TI
X1C=X1
X2C=X2
X3C=X3
X4C=X4
DO 2 I=1,4
A=1.+3.*X1C-X2C-X4C
XA=XAI+X1C
XP=XPI+X2C-X3C
XH=XHI+3.*X1C-X2C-(N-3.)*X3C/3.-N/3.*X4C
XN=XNI-(X1C+X2C+X4C)
E1=A11(T)
E2=A21(T)
E3=A12(T)

```

```

E4=A22(T)
E5=A31(T)
C1=F1(P)
C2=F2(P)
C3=F3(A)
C4=F4(A)
A =AD(1,1)*T+AD(2,1)
A1=AD(1,2)*T+AD(2,2)
A2=AD(1,3)*T+AD(2,3)
A3=AD(1,4)*T+AD(2,4)
A4=AD(1,5)*T+AD(2,5)
CP=A +A1*X1C+A2*X2C+A3*X3C+A4*X4C
IF(I.EQ.1) CALL DTRI
K(I,1)=C1
K(I,2)=C2
K(I,3)=C3
K(I,4)=C4
K(I,5)=F5(C1)
IF(I.EQ.4) GO TO 2
X1C=X1+H*K(I,1)/C(I)
X2C=X2+H*K(I,2)/C(I)
X3C=X3+H*K(I,3)/C(I)
X4C=X4+H*K(I,4)/C(I)
T=TI+H*K(I,5)/C(I)
2 CONTINUE
DO 3 I=1,5
3 PHI(I)=(K(1,I)+K(2,I)*2.+K(3,I)*2.+K(4,I))/6.
X1=X1+H*PHI(1)
X2=X2+H*PHI(2)
X3=X3+H*PHI(3)
X4=X4+H*PHI(4)
TI=TI+H*PHI(5)
1 CONTINUE
A=1.+3.*X1.X2-X4
XA=XAI+X1
XN=XNI*(X1+X2+X4)
XH=XHI+3.*X1-X2*(N-3.)*X3/3.-N*X4/3.
XP=XPI+X1.X2
T=TI
F1=A11(T)
F2=A21(T)
F3=A12(T)
F4=A22(T)
F5=A31(T)
C1=F1(P)
C2=F2(P)
C3=F3(A)
C4=F4(A)
A1=AD(1,1)*T+AD(2,1)
A1=AD(1,2)*T+AD(2,2)
A2=AD(1,3)*T+AD(2,3)
A3=AD(1,4)*T+AD(2,4)
A4=AD(1,5)*T+AD(2,5)
CP=A1*X1+A2*X2+A3*X3+A4*X4
CP=CP+A0

```

```

FU(IJ,1)=C1
FU(IJ,2)=C2
FU(IJ,3)=C3
FU(IJ,4)=C4
FU(IJ,5)=FS(C1)/ABC
CALL DERI
WRITE (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INCL)
RETURN
END

```

IBFTC SUB2

SUBROUTINE DERI

THIS SUBROUTINE CALCULATES DERIVATIVES OF MODEL EQUATIONS

```

COMMON /BL2/ E1,E2,E3,E4,E5,A,DD,B,F,C,IC,CP,C1,C2,C3,C4,T
COMMON /BL4/ D
COMMON /BL7/ A1,A2,A3,A4,P,FT
COMMON /BL9/ ABC
COMMON /BL10/ N
COMMON /BL17/ AD(2,5)
DIMENSION D(5,5,51),G(5)
REAL N
IC=IC+1
B1=E1*P/(FT*A**2)
B4=P**3*C**2/(A**3*E2)
D(1,1,IC)=B1*(-4-3.*B-B4*(A*(C+9.*DD)-12.*C*DD))
D(1,2,IC)=B1*(-A+B-B4*(-3.*A*DD+4.*C*DD))
D(1,3,IC)=B1*B4*DD*(N-3.)*A
D(1,4,IC)=B1*(B-A-B4*(-N*DD*A+4.*DD*C))
D(1,5,IC)=B1*A*B*34750./T**2+P**4*DD*C**3*EXP(11295./T-22.94)*11295.
15./(A**4*T**2*FT)
B1=E1*P/(FT*A**2)
B4=P/A
D(2,1,IC)=B1*(B4*(-A*C+B.*B*A*6.*B*C)+3.*E/E4)
D(2,2,IC)=B1*(B4*(-A*C-B*A+2.*B*C)-(A+E)/E4)
D(2,3,IC)=B1*(-B4*(N-3.)*B*A/3.+A/E4)
D(2,4,IC)=B1*(B4*(-A*C-N*A*B/3.+2.*B*C)-E/E4)
D(2,5,IC)=B1*P*B*C*59600./T**2-EXP(43.1-67600./T)*P*E*67600./(T**2
1*FT*A)
B1=E5/(FT*A**2)
D(3,1,IC)=-B1*B.*E
D(3,2,IC)=B1*(A+E)
D(3,3,IC)=-B1*A
D(3,4,IC)=B1*E
D(3,5,IC)=B1*A*E*62300./T**2
D(4,1,IC)=B1*(-4-3.*B)
D(4,2,IC)=B1*(-A+B)
D(4,3,IC)=0.
D(4,4,IC)=B1*(-A+B)
D(4,5,IC)=B1*A*B*62300./T**2
DO 1 J=1,5
1 G(J)=(-D(1,J,IC)*91500.+D(2,J,IC)*19000.+(N-3.)*D(3,J,IC)*8100.+D(
14,J,IC)*N*7433.)*CP
B1=-C1*91500.+C2*19000.+C3*(N-3.)*8100.+C4*N*7433.
D(5,1,IC)=(G(1)-B1*A1)/CP**2

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D(5,2,IC)=(G(2)-B1*A2)/CP**2
D(5,3,IC)=(G(3)-B1*A3)/CP**2
D(5,4,IC)=(G(4)-B1*A4)/CP**2
D(5,5,IC)=G(5)/CP**2-B1*(AD(1,1)+AD(1,2)+AD(1,3)+AD(1,4)+AD(1,5))/CP**2
1CP**2
DO 2 J=1,4
D(J,5,IC)=D(J,5,IC)+ABC
2 D(5,J,IC)=D(5,J,IC)/ABC
RETURN
END
IBFTC SUB3
SUBROUTINE LAMS
C
C THIS SUBROUTINE INTEGRATE THE SYSTEM VARIATIONAL EQUATIONS
C
COMMON /BL4/ D
COMMON/BL5/ LI
COMMON /BL6/ C(5),F
COMMON /BL8/ INC,INCL,INC2
REAL LI(5),L(5),K(4,5)
DIMENSION D(5,5,51)
DIMENSION IA(4)
IC=INC
IA(1)=0
IA(2)=1
IA(3)=1
IA(4)=2
DO 8 II=1,INC2
DO 7 I=1,5
7 L(I)=LI(I)
DO 9 IJ=1,4
IC1=IC-IA(IJ)
DO 10 I=1,5
K(IJ,I)=0
DO 10 J=1,5
10 K(IJ,I)=K(IJ,I)-L(J)*D(J,I,IC1)
IF(IJ.EQ.4) GO TO 9
DO 11 I=1,5
IF(ABS(L(I)).GT.100+9) GO TO 15
11 L(I)=LI(I)+F*K(IJ,I)/C(IJ)
9 CONTINUE
DO 12 I=1,5
12 LI(I)=LI(I)+H*(K(1,I)+K(2,I)*2.+2.*K(3,I)+K(4,I))/6.
8 IC=IC+2
RETURN
15 PRINT
1 FORMAT(//1X,* VALUES ARE OVER FLOWING IN LAMS*//)
STOP
END
IBFTC SUB4
SUBROUTINE LAMA
C
C THIS SUBROUTINE IS TO INTEGRATE THE ADJOINT EQUATIONS
C
COMMON /BL4/ D

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COMMON /BL5/ LI
COMMON /BL6/ C(3),F
COMMON /BL8/ INC,INCL,INC2
REAL LI(5),L(5),K(4,5)
DIMENSION D(5,5,51)
  DIMENSION IA(4)
  IC=1
  IA(1)=1
  IA(2)=1
  IA(3)=1
  IA(4)=2
  DO 8 II=1,INC2
  DO 7 I=1,5
7    L(I)=LI(I)
  DO 9 IJ=1,4
  IC1=IC+IA(IJ)
  DO 10 I=1,5
  K(IJ,I)=0.
  DO 11 J=1,5
10   K(IJ,I)=K(IJ,I)+L(J)*D(I,J,IC1)
  IF(IJ.EQ.4) GO TO 6
  DO 11 I=1,5
  IF(ABS(L(I)).GT.1.E+9) GO TO 15
11   L(I)=LI(I)+F*K(IJ,I)/C(IJ)
  9    CONTINUE
  DO 12 I=1,5
12   LI(I)=LI(I)+H*(K(1,I)+K(2,I)*2.+2.*K(3,I)+K(4,I))/6.
  8    IC=IC+2
  RETURN
15   PRINT1
  1    FORMAT(///1X,* VALUES ARE OVER FLOWING IN LAMA*//)
  STOP
  END
IBFTC SUB5
  SUBROUTINE CPT1(TT,IC3)
C
C   THIS SUBROUTINE CALCULATES GRADIENT VECTOR FOR DECISION VARIABLES
C
COMMON /BL1/ X1,X2,X3,X4
COMMON /BL4/ D
COMMON /BL5/ LI
COMMON /BL6/ C(3),H
COMMON /BL7/ IJ,FL(5,5)
COMMON /BL8/ INC,INCL,INC2
COMMON /BL10/ N
  COMMON /BL11/ DD(4),C1,C2,E1,B2,B3,DIV,IR,IR1
COMMON /BL13/ TIN(5),WIN(5)
COMMON /BL14/ WC,A
  DIMENSION WC(5)
  DIMENSION TT(5)
  DIMENSION D(5,5,51),DI(6,6,3),AA(2,3)
  REAL LA(5,5,5),LS(5,5,5),LAA(5,5,2),NU(2),LI(5),N
  REWIND 1
  DO 2 IJ=1,IR
  READ (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INCL)

```

```

H=WC(IJ)/FLOAT(INC1)
DO 3 I=1,4
DO 4 J=1,5
4 LI(J)=0.
LI(I)=1.
CALL LAMS
DO 3 J=1,5
3 LS(IJ,I,J)=LI(J)
2 CONTINUE
REWIND 1
DO 6 IJ=1,IR
READ (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
H=WC(IJ)/FLCAT(INC2)
IJK=1
IF(IJ.EQ.1) IJK=5
DO 7 I=IJK,5
DO 8 J=1,5
8 LI(J)=0.
LI(I)=1.
CALL LAMA
DO 7 J=1,5
7 LA(IJ,I,J)=LI(J)
6 CONTINUE
LAA(IR,1,1)=1.
LAA(IR,1,2)=1./A+(B1+X1)*B./A**2
LAA(IR,2,1)=0.
LAA(IR,2,2)=-(B1+X1)*B3/A**2
LAA(IR,3,1)=0.
LAA(IR,3,2)=-(B1+X1)*(-1.+N/15.+(N-3.)*B3/3.)/A**2
LAA(IR,4,1)=0.
LAA(IR,4,2)=-(B1+X1)*(-1.+N/15.+N*B3/3.)/A**2
LAA(IR,5,1)=0.
LAA(IR,5,2)=0.
DO 22 JI=1,IR1
IJ=IR+1-JI
DO 9 I=1,5
SC=0.
SD=0.
DO 10 J=1,4
10 SC=SC+LAA(IJ,J,1)*LA(IJ,I,J)
SD=SD+LAA(IJ,J,2)*LA(IJ,I,J)
LAA(IJ-1,I,1)=SC
9 LAA(IJ-1,I,2)=SD
LAA(IJ,5,1)=LAA(IJ-1,5,1)
LAA(IJ,5,2)=LAA(IJ-1,5,2)
22 CONTINUE
SC=0.
SD=0.
DO 11 J=1,4
11 SC=SC+LAA(1,J,1)*LA(1,5,J)
SD=SD+LAA(1,J,2)*LA(1,5,J)
LAA(1,5,1)=SC
LAA(1,5,2)=SD
DO 12 IJ=1,IR
SD=0.

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```

SC=0.
DO 13 I=1,4
SC=SC+FU(IJ,I)*LAA(IJ,I,1)
13 SD=SD+FU(IJ,I)*LAA(IJ,I,2)
DI(IJ,6,1)=-SC
DI(IJ,6,2)=-SD
DI(IJ,6,3)=-1.
DI(IJ,5,1)=LAA(IJ,5,1)
DI(IJ,5,2)=LAA(IJ,5,2)
12 DI(IJ,5,3)=0.
IC1=IR
IC2=1
IC3=1
65 DO 14 I=1,4
DO 14 J=1,3
14 DI(2,I,J)=LS(1,I,5)*DI(1,5,J)+FU(1,I)*DI(1,6,J)
DO 15 IJ=2,IR
DO 15 I=1,4
SC=0.
SD=0.
SE=0.
DO 17 J=1,5
SF=LS(IJ,I,J)
SC=SC+DI(IJ,J,1)*SF
SD=SD+DI(IJ,J,2)*SF
SE=SE+DI(IJ,J,3)*SF
17 CONTINUE
SF=FU(IJ,I)
DI(IJ+1,1,1)=SC+DI(IJ,6,1)*SF
DI(IJ+1,1,2)=SD+DI(IJ,6,2)*SF
DI(IJ+1,1,3)=SE+DI(IJ,6,3)*SF
15 CONTINUE
AA(1,1)=DI(IR+1,1,1)
AA(1,2)=DI(IR+1,1,2)
AA(1,3)=DI(IR+1,1,3)
SC=0.
SD=0.
SE=0.
DO 16 I=1,4
SC=SC+DI(IR+1,I,1)*DD(I)
SD=SD+DI(IR+1,I,2)*DD(I)
SE=SE+DI(IR+1,I,3)*DD(I)
16 CONTINUE
AA(2,1)=SC
AA(2,2)=SD
AA(2,3)=SE
DT=AA(1,1)*AA(2,2)-AA(1,2)*AA(2,1)
IF(DT.EQ.0.) GO TO 18
NU(1)=(AA(1,3)*AA(2,2)-AA(2,3)*AA(1,2))/DT
NU(2)=(AA(1,1)*AA(2,3)-AA(2,1)*AA(1,3))/DT
DO 24 IJ=1,IR
DTE=DI(IJ,5,1)*NU(1)+DI(IJ,5,2)*NU(2)+DI(IJ,5,3)
DWC=DI(IJ,6,1)*NU(1)+DI(IJ,6,2)*NU(2)+DI(IJ,6,3)
TIN(IJ)=DTE
WIN(IJ)=DWC

```

```

24  CONTINUE
    IF(IC2.EQ.1) RETURN
    DO 61 IJ=1,IR
    IF(TT(IJ).EQ.1400.) GO TO 61
    IF(TT(IJ).EQ.1200.) GO TO 62
    GO TO 61
61  IF(TIN(IJ).LE.0.) GO TO 61
    GO TO 63
62  IF(TIN(IJ).GE.0.) GO TO 61
63  DI(IJ,5,1)=0.
    DI(IJ,5,2)=0.
    DI(IJ,5,3)=0.
    IC1=IC1+1
64  CONTINUE
    IF(IC1.EQ.IR) RETURN
    IF(IC1.GE.2) GO TO 64
    IC3=0
    RETURN
64  IC2=
    GO TO 65
18  PRINT2
20  FORMAT(//1X,* DETERMINENT IS ZERO*//)
    STOP
    END
IBFTC SUB6
    SUBROUTINE CPEV
C
C    SAME SUBROUTINE AS GIVEN IN SIMULATION PROGRAMME
C
ENTRY

```

JOB CGG136, TIME 0.9, PAGES 3, NAME ASHOK KUMAR SHARMA
 IBJOB
 IBFTC MAIN

PROGRAMME FOR MINIMIZATION OF OPERATING COST

IR IS NUMBER OF REACTORS IN SERIES
 C6PINR IS MOLE FRACTION OF C6 AND HIGHER HYDROCARBONS IN RECYCLE GAS
 FEED AND RECY ARE LB MOLES OF NAPHTHA FEED AND RECYCLE GAS PER HOUR
 PP IS PRESSURE OF THE INLET STREAM TO VARIOUS REACTORS
 TT AND WC ARE TEMPERATURES OF INLET STREAMS AND WEIGHT OF CATALYST IN
 EACH REACTOR
 INC IS NUMBER OF PARTS IN WHICH A REACTOR IS DIVIDED FOR INTEGRATION
 AB1 IS NUMBER OF MOLES OF NAPHTHA WHICH ARE USED AS BASIS OF CALCULATIONS
 FOR OPTIMIZATION
 AB2 IS SCALING FACTOR FOR OBJECTIVE FUNCTION
 ABC IS SCALING FACTOR FOR TEMPERATURE
 VALUES OF AB1 AND ABC ARE CHANGED DURING ITERATIONS AT SUITABLE PLACES
 THOUGH THE GIVEN STARTING VALUES HAVE BEEN FOUND TO BE GOOD, BUT IT IS
 ADVISED TO TRY OTHER STARTING VALUES FOR THESE FACTORS TO MINIMIZE TOTAL
 NUMBER OF ITERATIONS
 TD IS REFERENCE TEMPERATURE FOR FEED TO FIRST REACTOR OF THE SERIES
 DIV IS A FACTOR TO DECIDE MAGNITUDE OF CHANGES IN DECISION VARIABLES
 SO THAT ALL THE CONSTRAINTS ARE SATISFIED
 ITR3 IS MAXIMUM NUMBER OF ITERATIONS FOR WHICH THE PROGRAMME IS ALLOWED
 TO EXECUTE
 ER1 AND ER2 ARE AMOUNTS OF ERRORS ALLOWED +N CONSTRAINTS ONE AND TWO ON
 THE FINAL PRODUCT STREAM
 ER, IF THE CHANGE IN OBJECTIVE FUNCTION IS LESS THAN ER PROGRAMME IS
 TERMINATED AUTOMATICALLY AND THE SOLUTION VECTOR AT THIS PLACE IS PRINTED
 AS OPTIMIZED RESULTS
 IT IS ADVISED THAT MANY INITIAL SOLUTIONS BE TRIED TO ENSURE THE VALIDITY
 OF THE RESULTS

DATA CARDS

MOLE FRACTIONS OF RECYCLE GAS COMPONENTS STARTING FROM METHANE TO HEXANE
 AND HYDROGEN IN 10F8.4 FORMAT
 WEIGHT PERCENTAGES OF PARAFFINS(C6 TO C9), NAPHTHENES(C6 TO C9) AND
 AROMATICS(C6 TO C9) IN 10F8.4 FORMAT
 NUMBER OF REACTORS (I6)
 TEMPERATURE VECTOR, WEIGHT OF CATALYST VECTOR AND PRESSURE VECTOR (8F10.0)
 MOLE FRACTIONS OF C6 AND HIGHER COMPONENTS IN RECYCLE GAS (10F8.4)
 FEED AND RECY (8F10.0)
 THESE TT AND WC VALUES ARE USED AS A STARTING VECTOR FOR OPTIMIZATION
 AT THESE VALUES ALL THE CONSTRAINTS SHOULD BE SATISFIED

COMMON /BL1/ X1,X2,X3,X4
 COMMON /BL3/ A1,A2,A3,A4,P,FT
 COMMON /BL6/ C(3),H
 COMMON /BL7/ IJ,FU(5,5)
 COMMON /BL8/ INC,INC1,INC2
 COMMON /BL9/ ABC
 COMMON /BL10/ N
 COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
 COMMON /BL12/ TI,XAI,XPI,XNI,XHI,XHYI,A

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COMMON /BL12/ TIN(5),WIN(5)
COMMON /BL14/ WC,A
COMMON /BL15/ CPA(2),CPN(2),CPP(2),CPH(2),CPHY(2),CPHYI(2)
COMMON /BL16/ XPF,XNF,XAF,XFYR,XH2R,MWF,MWRE
COMMON /BL17/ AD(2,5)
COMMON /BL20/ XDUT
COMMON /BL21/ XIN
DIMENSION PP(5),WC(5),TT(5)
DIMENSION AA(5,3),AAA(5,2),PT(5),PW(5)
DIMENSION XINR(3,4),TOUT(5),XIN(5,6),XDUT(5,6)
DIMENSION ABD(5),ACC(5)
REAL N,MWF,MWRE
DATA PT,PW/6H T1 ,6H T2 ,6H T3 ,6H T4 ,6H T5 ,6H W1 ,
16H W2 ,6H W3 ,6H W4 ,6H W5 /
CALL CP3V
AB1=1.0
AB2=1.0
ABC=1.0
TD=120.0
ER=5.0
ER1=.0005
ER2=.0005
IC4=0
ITR3=5
DIV=.25
DIV1=DIV
READ 60,IR
READ 61,(TT(I),WC(I),PP(I),I=1,IR)
61 FORMAT(8F10.0)
60 FORMAT(I6)
IR1=IR-1
SC1=1.0E+32
C(1)=2.0
C(2)=2.0
C(3)=1.0
READ 61,FEED,RECY
READ 61,C6PINR
AFT=FEED+RECY
A=FEED
DO 18 I=1,IR
18 WC(I)=WC(I)*AB1/A
PRINT3
PRINT2
3 FORMAT(1H1)
2 FORMAT(////10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,30X,*FEED DATA*,30
1X,1H*/10X,1H*,70X,1H*/10X,72(1H*)/10X,1H*,70X,1H*/10X,1H*,70X,1H*)
PRINT17,FEED,RECY,MWF,MWRE
17 FORMAT(10X,1H*,20X,*NAPHTHA FEED LB MOLE/HR =*,F8.1,17X,1H*/10X,1H
1*,70X,1H*/10X,1H*,21X,*RECYCLE GAS LB MOLE/HR =*,F8.1,17X,1H*/10X,
21H*,70X,1H*/10X,1H*,17X,*LB MOLECULAR WT OF NAPHTHA =*,F8.1,17X,1H
3*/10X,1H*,70X,1H*/10X,1H*,12X,*LB MOLECULAR WT OF RECYCLE GAS =*,F
48.1,17X,1H*/10X,1H*,70X,1H*)
DD(1)=XAF*FEED+RECY*C6PINR
DD(2)=XNF*FEED
DD(3)=XPF*FEED

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```

CC(4)=XHYR*RECY-RECY*C6PINR
A=XH2R*RECY
PRINT19,CC,A,PP(1)
19  FORMAT(10X,1H*,23X,*AROMATICS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,7
10X,1H*/10X,1H*23X,*NAPHTHENES LB MOLE/HR =*,F8.1,17X1H*/10X1H*70X1
2H*/10X1H*23X*PARAFFINS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,70X,1H*/1
30X,1H*,23X,*HYDROCARBONS LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*,70X,1H
4*,/10X,1H*,24X,*HYDROGEN LB MOLE/HR =*,F8.1,17X,1H*/10X,1H*70X,1H*
5/10X,1H*,27X,*INLET PRESSURE (ATM) =*,F8.1,17X,1H*/10X,1H*,70X,1H*
6/10X,1H*,70X,1H*/10X,72(1H*))
FT=FRED+RECY
CONV=FRED/(FRED+RECY)
XAI=XAF+CONV+RECY*C6PINR/FT
XPI=XPF+CONV
XNI=XNF+CONV
XHI=XH2R*RECY/FT
XHYI=XHYR*RECY/FT-RECY*C6PINR/FT
A=FRED
FT=AB1+RECY*AB1/A
N=(MWF+2.*XNF+A6.*XAF)/14.
PRINT22,(PT(1),I=1,IR),(PW(I),I=1,IR)
PRINT62
62  FORMAT(95X,6X,*C1*,5X,*C2*,4X,*OBJECTIVE FUNC*)
22  FORMAT(1H1/10X,*ITER *,A6,9(2X,A6)/)
XN=XNI
XP=XPI
XH=XHI
XA=XAI
DO 31 I=1,2
A1=CPA(I)*XA+CPP(I)*XP+CPN(I)*XN+CPH(I)*XH+CPHYI(I)*XHYI
A1=CPA(I)-CPN(I)+3.*CPH(I)
A2=CPP(I)-CPN(I)-CPH(I)
A3=CPHYI(I)*N/3.-CPP(I)-(N-3.)*CPH(I)/3.
A4=CPHYI(I)*N/3.-CPN(I)-CPH(I)*N/3.
AD(I,1)=A1
AD(I,2)=A2
AD(I,3)=A2
AD(I,4)=A3
AD(I,5)=A4
31  CONTINUE
ITS=
INC=50
INCL=INC+1
INC2=INC/2
DO 26 ITR4=1,ITR3
X1=0.
X2=0.
X3=0.
X4=0.
REWIND 1
DO 5 IJ=1,IR
XINR(IJ,1)=X1
XINR(IJ,2)=X2
XINR(IJ,3)=X3
XINR(IJ,4)=X4

```



```

P=PP(IJ)
TI=TT(IJ)
H=WC(IJ)/FLCAT(INC)
AA(IJ,1)=WC(IJ)*FEED/AB1
AA(IJ,2)=TI
CALL SIMULA
TOUT(IJ)=TI
AA(IJ,3)=TI
AA(IJ,4)=AFT*(X1+XA)
AA(IJ,5)=AFT*(X1I+(X1+X2+X4))
AA(IJ,6)=AFT*(XP+X2+X3)
AA(IJ,7)=AFT*(XH+B.*X1-X2-(N-B.)*X3/3.-N*X4/3.)
AA(IJ,8)=AFT*(XHYI+(X3+X4)*N/2.)
5 CONTINUE
IF(ITR4.EQ.1) C1=X1
B1=XAI
B2=XAI+XNI+XPI
B3=.1/34
A=B2*X2*B.*B1+X2*B3+X3*(B3*(N-B.)/3.-(15.-N)/15.)+X4*(B3*N/3.-(15.-N)/15.)
CO2=(B1+X1)/A
IF(ITR4.EQ.1) C2=CO2
PRINT23, ITR4, (TT(IJ), IJ=1, IR), (AA(IJ,1), IJ=1, IR)
23 FORMAT(1X, I2, 1F8.1)
IF(ABS(C1-X1).GT.FR1) GO TO 6
IF(ABS(C2-CC2).GT.FR2) GO TO 6
DIV=DIV1
IF(IT5.EQ.1) GO TO 11
IF(IC4.EQ.1) GO TO 46
CALL OBJE(T1, TOUT, XINR, AB1, AB2, TU, SC)
SC=SC*AB2*AFT
PRINT46, X1, CO2, SC
46 FORMAT(95X, 2F1.4, 4.4)
IF(SC.GT.SC1) GO TO 47
IF((SC1-SC).LT.FR) GO TO 20
GO TO 42
47 AB1=AB1+.1
ABC=ABC+2.
DIV=DIV1
IC4=1
PRINT7
7 FORMAT(100X, * FOUND +VE*)
DO 44 IJ=1, IR
TT(IJ)=AAA(IJ, 2)
44 WC(IJ)=AAA(IJ, 1)*AB1/FEED
FT=AB1+RECY*AB1/FEED
GO TO 26

```

```

42 SC1=SC
46 CALL OBJED(TT,TCUT,XINR,AB1,AB2,TC)
   IC4=0
   DD(1)=1.+3.*B3*C2
   DD(2)=-B3*C2
   DD(3)=C2*(15.-N)/15.-B3*C2*(N-3.)/3.
   DD(4)=C2*(15.-N)/15.-B3*C2*(N-3.)/3.
   DD(1)=C2*A+(B1+X1)*(DD(1)-1.)
   DD(2)=DD(2)*(B1+X1)
   DD(3)=DD(3)*(B1+X1)
   DD(4)=DD(4)*(B1+X1)
   IF(ITR4.EQ.0) GO TO 34
   CALL OPTI(TT,IC3)
   IF(IC3.EQ.0) GO TO 27
   D2=C02
   D1=X1
   DO 16 IJ=1,IR
   DO 16 I=1,8
16  AAA(IJ,I)=AA(IJ,I)
   GO TO 41
6   PRINT8
8   FORMAT(10X,'CONST VIOLATED')
   IT5=1
   DIV=DIV*2.
   DO 45 IJ=1,IR
   TT(IJ)=AAA(IJ,2)
45  WC(IJ)=AAA(IJ,1)*AB1/FRED
41  DO 35 IJ=1,IR
   ABD(IJ)=1.
   TIC=TT(IJ)+TIN(IJ)*ABC/DIV
   IF(TIC.GT.1460.) GO TO 36
   IF(TIC.LT.1260.) GO TO 37
   GO TO 35
36  ABD(IJ)=(1460.-TT(IJ))*DIV/(TIN(IJ)*ABC)
   AC2(IJ)=1460.
   GO TO 35
37  ABD(IJ)=(1260.-TT(IJ))*DIV/(TIN(IJ)*ABC)
   AC2(IJ)=1260.
35  CONTINUE
   IC1=1
   DO 38 IJ=2,IR
   IF(ABD(IJ).LT.ABD(IC1)) IC1=IJ
38  CONTINUE
   AB3=ABD(IC1)
   AC1=0.
   IT1=0
   DO 39 IJ=1,IR
   TT(IJ)=TT(IJ)+TIN(IJ)*AB3*ABC/DIV
   WC(IJ)=WC(IJ)+WIN(IJ)*AB3/DIV
   IF(WC(IJ).GT.0.) GO TO 39
   IF(AC1.LT.WC(IJ)) GO TO 39
   IT1=IJ
   AC1=WC(IJ)
39  CONTINUE

```

```

IF(AB3.LT.1.) TT(IC1)=AC2(IC1)
IF(IT1.EQ. ) GO TO 26
AB4=WC(IT1)/(WIN(IT1)*AB3/DIV)
DO 48 IJ=1,IR
TT(IJ)=TT(IJ)-TIN(IJ)*AB3*AB4*ABC/DIV
48 WC(IJ)=WC(IJ)-WIN(IJ)*AB3*AB4/DIV
ITS=1
26 CONTINUE
34 PRINT33
33 FORMAT(//1 X,*ITERATION LESS FEED PROGRAMME AGAIN*//)
GO TO 1
27 PRINT22
28 FORMAT(///5X,*LESS THAN TWO TEMPERATURES ARE AWAY FROM BOUNDARY *)
GO TO 1
2 CONTINUE
DO 9 IJ=1,IR
DO 9 I=1,8
9 AA(IJ,I)=AAA(IJ,I)
X1=D1
CO2=D2
GO TO 1
1 PRINT21
21 FORMAT(1H1,5X,*OPTIMIZED RESULTS ARE*//)
PRINT14
14 FORMAT(/////1 X,*REACTOR WT CATA T IN R T OUT R AROMAT NAPHTH
1 PARAFFIN HE HYDROC*//)
DO 12 I=1,IR
PRINT13,I,(AA(I,J),J=1,8)
13 FORMAT(1 X,I4,F12.1,F8.1,F9.1,F7.1,F8.1,F9.1,F10.1,F8.1/)
12 CONTINUE
PRINT15,CO2
15 FORMAT(//1 X,*PERCENTAGE OF AROMATICS IN C5+ AT OUTLET=*,F6.3//)
STOP
END

IBFTC SUB1
SUBROUTINE SIMULA
C
C SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
IBFTC SUB2
SUBROUTINE DER1
C
C SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
IBFTC SUB3
SUBROUTINE LAMS
C
C SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
IBFTC SUB4
SUBROUTINE LAMA
C
C SAME SUBROUTINE AS GIVEN IN PROGRAMME FOR MINIMIZING WEIGHT OF CATALYST
C
IBFTC SUB5
SUBROUTINE CPT1(TT,IC3)

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COMMON /BL1/ X1,X2,X3,X4
COMMON /BL4/ D
COMMON /BL5/ LI
COMMON /BL6/ C(3),F
COMMON /BL7/ IJ,FL(5,5)
COMMON /BL8/ INC,INC1,INC2
COMMON /BL10/ N
COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
COMMON /BL12/ TI(5),WIN(5)
COMMON /BL14/ WC,A
COMMON /BL20/ TOUT
COMMON /BL21/ KIN
DIMENSION XIN(5,6),XCUT(5,4)
DIMENSION D(5,3,5),DI(6,6,3),AA(2,3)
DIMENSION WC(5)
DIMENSION TT(5)
REAL LAS(5,3)
REAL LA(5,5,5),LS(5,5,5),LAA(5,5,3),NU(2),LI(5),N
REWIND 1
DO 2 IJ=1,IR
READ (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
H=-WC(IJ)/FLOAT(INC2)
DO 3 I=1,4
DO 4 J=1,5
4 LI(J)=0.
LI(I)=1.
CALL LAMS
DO 3 J=1,5
3 LS(IJ,I,J)=LI(J)
2 CONTINUE
REWIND 1
DO 6 IJ=1,IR
READ (1) (((D(I,J,JM),I=1,5),J=1,5),JM=1,INC1)
H=WC(IJ)/FLOAT(INC2)
IJK=1
IF(IJ.EQ.1) IJK=5
DO 7 I=IJK,5
DO 8 J=1,5
8 LI(J)=0.
LI(I)=1.
CALL LAMA
DO 7 J=1,5
7 LA(IJ,I,J)=LI(J)
6 CONTINUE
LAA(IR,1,1)=1.
LAA(IR,1,2)=1./A+(B1+X1)*B3*B3/A**2
LAA(IR,2,1)=0.
LAA(IR,2,2)=- (B1+X1)*B3/A**2
LAA(IR,3,1)=0.
LAA(IR,3,2)=- (B1+X1)*(-1.+N/15.+(N-3.)*B3/3.)/A**2
LAA(IR,4,1)=0.
LAA(IR,4,2)=- (B1+X1)*(-1.+N/15.+N*B3/3.)/A**2
LAA(IR,5,1)=0.
LAA(IR,5,2)=0.
LAA(IR,1,3)=0.

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LAA(IR,2,3)=0
LAA(IR,3,3)=0
LAA(IR,4,2)=0
LAA(IR,5,3)=0
DO 22 JI=1,IR1
IJ=IR+1-JI
DO 9 I=1,5
SC=0
SD=0
SE=0
DO 10 J=1,5
SE=LAA(IJ,J,1)*LA(IJ,I,J)+SE
SC=SC+LAA(IJ,J,1)*LA(IJ,I,J)
10 SD=SD+LAA(IJ,J,2)*LA(IJ,I,J)
LAA(IJ-1,I,3)=SE-XIN(IJ,I)
LAA(IJ-1,I,1)=SC
9 LAA(IJ-1,I,2)=SD
SE=0
LAA(IJ-1,5,1)=0
LAA(IJ-1,5,2)=0
LAA(IJ-1,5,3)=-XOUT(IJ-1,5)
LAS(IJ,1)=SC
LAS(IJ,2)=SD
LAS(IJ,3)=SE
22 CONTINUE
SC=0
SD=0
SE=0
DO 11 J=1,5
SE=SE+LAA(1,J,3)*LA(1,5,J)
SC=SC+LAA(1,J,1)*LA(1,5,J)
11 SD=SD+LAA(1,J,2)*LA(1,5,J)
LAS(1,1)=SC
LAS(1,2)=SD
LAS(1,3)=SE
DO 12 IJ=1,IR
SE=0
SC=0
SD=0
DO 13 I=1,5
SE=SE+FU(IJ,I)*LAA(IJ,I,3)
SC=SC+FU(IJ,I)*LAA(IJ,I,1)
13 SD=SD+FU(IJ,I)*LAA(IJ,I,2)
DI(IJ,6,1)=-SC
DI(IJ,6,2)=-SD
DI(IJ,6,3)=-XIN(IJ,6)-SE
DI(IJ,5,1)=LAS(IJ,1)
DI(IJ,5,2)=LAS(IJ,2)
12 DI(IJ,5,3)=LAS(IJ,3)-XIN(IJ,5)
IC1=IR
IC2=1
IC3=1
65 DO 14 I=1,4
DO 14 J=1,3
14 DI(2,I,J)=LS(1,I,5)*DI(1,5,J)+FU(1,I)*DI(1,6,J)

```

```

DO 15 IJ=2,IR
DO 15 I=1,4
SC=0.
SD=0.
SE=0.
DO 17 J=1,5
SF=LS(IJ,I,J)
SC=SC+DI(IJ,J,1)*SF
SD=SD+DI(IJ,J,2)*SF
SE=SE+DI(IJ,J,3)*SF
17 CONTINUE
SF=FU(IJ,I)
DI(IJ+1,1,1)=SC+DI(IJ,6,1)*SF
DI(IJ+1,1,2)=SD+DI(IJ,6,2)*SF
DI(IJ+1,1,3)=SE+DI(IJ,6,3)*SF
15 CONTINUE
AA(1,1)=DI(IR+1,1,1)
AA(1,2)=DI(IR+1,1,2)
AA(1,3)=-DI(IR+1,1,3)
SC=0.
SD=0.
SE=0.
DO 16 I=1,4
SC=SC+DI(IR+1,I,1)*DD(I)
SD=SD+DI(IR+1,I,2)*DD(I)
SE=SE+DI(IR+1,I,3)*DD(I)
16 CONTINUE
AA(2,1)=SC
AA(2,2)=SD
AA(2,3)=-SE
DT=AA(1,1)*AA(2,2)-AA(1,2)*AA(2,1)
IF(DT.EQ.0.) GO TO 13
NU(1)=(AA(1,3)*AA(2,2)-AA(2,3)*AA(1,2))/DT
NU(2)=(AA(1,2)*AA(2,3)-AA(2,1)*AA(1,3))/DT
DO 24 IJ=1,IR
DTE=DI(IJ,5,1)*NU(1)+DI(IJ,5,2)*NU(2)+DI(IJ,5,3)
DWC=DI(IJ,6,1)*NU(1)+DI(IJ,6,2)*NU(2)+DI(IJ,6,3)
TIN(IJ)=DTE
WIN(IJ)=DWC
24 CONTINUE
IF(IC2.EQ.0.) RETURN
DO 60 IJ=1,IR
IF(TT(IJ).EQ.1440.) GO TO 61
IF(TT(IJ).EQ.1250.) GO TO 62
GO TO 5
61 IF(TIN(IJ).LE.0.) GO TO 60
GO TO 62
62 IF(TIN(IJ).GE.0.) GO TO 60
63 DI(IJ,5,1)=0.
DI(IJ,5,2)=0.
DI(IJ,5,3)=0.
IC1=IC1-1
60 CONTINUE
IF(IC1.EQ.IR) RETURN
IF(IC1.GE.2) GO TO 64

```

```

        IC3=0
        RETURN
64      IC2=0
        GO TO 65
18      PRINT2
26      FORMAT(1X,* DETERMINENT IS ZERO*)
        STOP
        END
IBFTC SUB6
        SUBROUTINE CBJ6(TT,TCUT,XINR,AB1,AB2,TO,SC)
C
C      THIS SUBROUTINE CALCULATE THE OBJECTIVE FUNCTION
C
        COMMON /BL14/ WC,A
        COMMON /BL17/ AD(2,5)
        COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
        COMMON /BL21/ XIN
        DIMENSION TT(5),WC(5),XIN(5,6),TOUT(5),XINR(5,4)
        AX=.456*24.*36./((.9*AB1*AB2)
        SD=AD(1,1)*(TT(1)**2-TCUT**2)/2.+AD(2,1)*(TT(1)-TO)
        SE=0.
        SC=WC(1)*14./(.9*AB1*AB2)
        DO 45 IJ=2,IR
        SC=SC+WC(IJ)*14./(.9*AB1*AB2)
        SD=SD+AD(1,1)*(TT(IJ)**2-TCUT(IJ-1)**2)/2.+AD(2,1)*(TT(IJ)-TOUT(IJ
1))
        DO 46 I=1,4
46      SE=SE+(AD(1,I+1)*(TT(IJ)**2-TCUT(IJ-1)**2)/2.+AD(2,I+1)*(TT(IJ)-TO
1UT(IJ-1)))*XINR(IJ,I)
45      CONTINUE
        SC=SC*366.872/2439.2
        SC=SC+(SC+SE)*AX
        SC=SC*1.
        RETURN
        END
IBFTC SUB7
        SUBROUTINE CBJ7(TT,TCUT,XINR,AB1,AB2,TO)
C
C      THIS SUBROUTINE IS TO CALCULATE THE DERIVATIVES OF THE OBJECTIVE FUNCTION
C
        COMMON /BL17/ AD(2,5)
        COMMON /BL9/ ABC
        COMMON /BL11/ DD(4),C1,C2,B1,B2,B3,DIV,IR,IR1
        COMMON /BL14/ WC,A
        COMMON /BL20/ XOUT
        COMMON /BL21/ XIN
        DIMENSION XOUT(5,6)
        DIMENSION TT(5),WC(5),XIN(5,6),TOUT(5),XINR(5,4)
        DO 41 I=1,4
41      XIN(1,I)=0.
        AX=.456*24.*36./((1000000.*AB2)
        XIN(1,5)=(AD(1,1)*TT(1)+AD(2,1))*AX
        XIN(1,5)=XIN(1,5)*ABC
        XIN(1,6)=14./(.9*AB1*AB2)
        XIN(1,6)=XIN(1,6)*366.872/2439.2

```